Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 09:32 PM EDT

PDB ID	:	2F6I
Title	:	Crystal structure of the ClpP protease catalytic domain from Plasmodium falciparum
Authors	:	Mulichak, A.; Loppnau, P.; Bray, J.; Amani, M.; Vedadi, M.; Wasney, G.; Finerty, P.; Sundstrom, M.; Weigelt, J.; Edwards, A.; Arrowsmith, C.; Hui, R.; Plotnikova, O.; Structural Genomics Consortium (SGC)
Deposited on	:	2005-11-29
Resolution	:	2.45 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 (i) 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 (1)) were used in the production of this report:

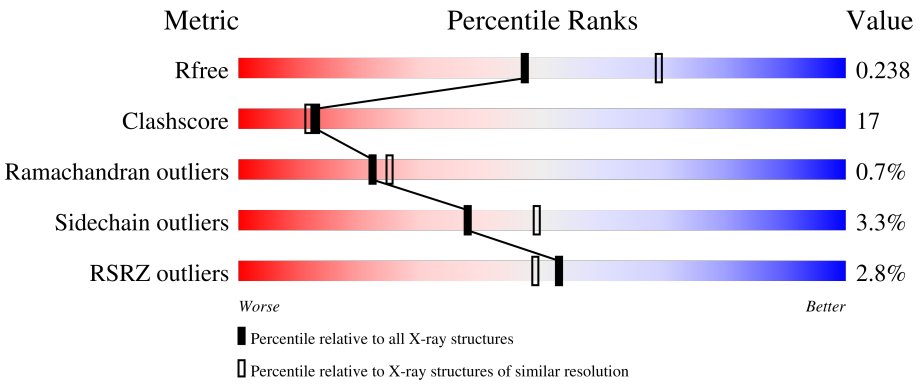
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 <=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	215	3% 64% 20% • 15%
1	B	215	% 55% 23% • 19%
1	C	215	4% 61% 22% • 15%
1	D	215	% 53% 31% • 15%
1	E	215	2% 57% 23% • 19%

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Mol	Chain	Length	Quality of chain
1	F	215	2% 59% 24% • 16%
1	G	215	2% 56% 24% • 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10189 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, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	182	1447	936	234	271	6	0	0	0
1	B	174	1387	898	223	260	6	0	0	0
1	C	183	1450	938	235	271	6	0	0	0
1	D	182	1434	927	233	269	5	0	0	0
1	E	175	1391	900	224	261	6	0	0	0
1	F	181	1434	927	232	270	5	0	0	0
1	G	178	1398	904	226	263	5	0	0	0

There are 161 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	MET	-	cloning artifact	UNP O97252
A	157	GLY	-	cloning artifact	UNP O97252
A	158	SER	-	cloning artifact	UNP O97252
A	159	SER	-	cloning artifact	UNP O97252
A	160	HIS	-	expression tag	UNP O97252
A	161	HIS	-	expression tag	UNP O97252
A	162	HIS	-	expression tag	UNP O97252
A	163	HIS	-	expression tag	UNP O97252
A	164	HIS	-	expression tag	UNP O97252
A	165	HIS	-	expression tag	UNP O97252
A	166	SER	-	cloning artifact	UNP O97252
A	167	SER	-	cloning artifact	UNP O97252
A	168	GLY	-	cloning artifact	UNP O97252
A	169	ARG	-	cloning artifact	UNP O97252
A	170	GLU	-	cloning artifact	UNP O97252

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Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ASN	-	cloning artifact	UNP O97252
A	172	LEU	-	cloning artifact	UNP O97252
A	173	TYR	-	cloning artifact	UNP O97252
A	174	PHE	-	cloning artifact	UNP O97252
A	175	GLN	-	cloning artifact	UNP O97252
A	176	GLY	-	cloning artifact	UNP O97252
A	177	HIS	-	cloning artifact	UNP O97252
A	178	MET	-	cloning artifact	UNP O97252
B	156	MET	-	cloning artifact	UNP O97252
B	157	GLY	-	cloning artifact	UNP O97252
B	158	SER	-	cloning artifact	UNP O97252
B	159	SER	-	cloning artifact	UNP O97252
B	160	HIS	-	expression tag	UNP O97252
B	161	HIS	-	expression tag	UNP O97252
B	162	HIS	-	expression tag	UNP O97252
B	163	HIS	-	expression tag	UNP O97252
B	164	HIS	-	expression tag	UNP O97252
B	165	HIS	-	expression tag	UNP O97252
B	166	SER	-	cloning artifact	UNP O97252
B	167	SER	-	cloning artifact	UNP O97252
B	168	GLY	-	cloning artifact	UNP O97252
B	169	ARG	-	cloning artifact	UNP O97252
B	170	GLU	-	cloning artifact	UNP O97252
B	171	ASN	-	cloning artifact	UNP O97252
B	172	LEU	-	cloning artifact	UNP O97252
B	173	TYR	-	cloning artifact	UNP O97252
B	174	PHE	-	cloning artifact	UNP O97252
B	175	GLN	-	cloning artifact	UNP O97252
B	176	GLY	-	cloning artifact	UNP O97252
B	177	HIS	-	cloning artifact	UNP O97252
B	178	MET	-	cloning artifact	UNP O97252
C	156	MET	-	cloning artifact	UNP O97252
C	157	GLY	-	cloning artifact	UNP O97252
C	158	SER	-	cloning artifact	UNP O97252
C	159	SER	-	cloning artifact	UNP O97252
C	160	HIS	-	expression tag	UNP O97252
C	161	HIS	-	expression tag	UNP O97252
C	162	HIS	-	expression tag	UNP O97252
C	163	HIS	-	expression tag	UNP O97252
C	164	HIS	-	expression tag	UNP O97252
C	165	HIS	-	expression tag	UNP O97252
C	166	SER	-	cloning artifact	UNP O97252

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Chain	Residue	Modelled	Actual	Comment	Reference
C	167	SER	-	cloning artifact	UNP O97252
C	168	GLY	-	cloning artifact	UNP O97252
C	169	ARG	-	cloning artifact	UNP O97252
C	170	GLU	-	cloning artifact	UNP O97252
C	171	ASN	-	cloning artifact	UNP O97252
C	172	LEU	-	cloning artifact	UNP O97252
C	173	TYR	-	cloning artifact	UNP O97252
C	174	PHE	-	cloning artifact	UNP O97252
C	175	GLN	-	cloning artifact	UNP O97252
C	176	GLY	-	cloning artifact	UNP O97252
C	177	HIS	-	cloning artifact	UNP O97252
C	178	MET	-	cloning artifact	UNP O97252
D	156	MET	-	cloning artifact	UNP O97252
D	157	GLY	-	cloning artifact	UNP O97252
D	158	SER	-	cloning artifact	UNP O97252
D	159	SER	-	cloning artifact	UNP O97252
D	160	HIS	-	expression tag	UNP O97252
D	161	HIS	-	expression tag	UNP O97252
D	162	HIS	-	expression tag	UNP O97252
D	163	HIS	-	expression tag	UNP O97252
D	164	HIS	-	expression tag	UNP O97252
D	165	HIS	-	expression tag	UNP O97252
D	166	SER	-	cloning artifact	UNP O97252
D	167	SER	-	cloning artifact	UNP O97252
D	168	GLY	-	cloning artifact	UNP O97252
D	169	ARG	-	cloning artifact	UNP O97252
D	170	GLU	-	cloning artifact	UNP O97252
D	171	ASN	-	cloning artifact	UNP O97252
D	172	LEU	-	cloning artifact	UNP O97252
D	173	TYR	-	cloning artifact	UNP O97252
D	174	PHE	-	cloning artifact	UNP O97252
D	175	GLN	-	cloning artifact	UNP O97252
D	176	GLY	-	cloning artifact	UNP O97252
D	177	HIS	-	cloning artifact	UNP O97252
D	178	MET	-	cloning artifact	UNP O97252
E	156	MET	-	cloning artifact	UNP O97252
E	157	GLY	-	cloning artifact	UNP O97252
E	158	SER	-	cloning artifact	UNP O97252
E	159	SER	-	cloning artifact	UNP O97252
E	160	HIS	-	expression tag	UNP O97252
E	161	HIS	-	expression tag	UNP O97252
E	162	HIS	-	expression tag	UNP O97252

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Chain	Residue	Modelled	Actual	Comment	Reference
E	163	HIS	-	expression tag	UNP O97252
E	164	HIS	-	expression tag	UNP O97252
E	165	HIS	-	expression tag	UNP O97252
E	166	SER	-	cloning artifact	UNP O97252
E	167	SER	-	cloning artifact	UNP O97252
E	168	GLY	-	cloning artifact	UNP O97252
E	169	ARG	-	cloning artifact	UNP O97252
E	170	GLU	-	cloning artifact	UNP O97252
E	171	ASN	-	cloning artifact	UNP O97252
E	172	LEU	-	cloning artifact	UNP O97252
E	173	TYR	-	cloning artifact	UNP O97252
E	174	PHE	-	cloning artifact	UNP O97252
E	175	GLN	-	cloning artifact	UNP O97252
E	176	GLY	-	cloning artifact	UNP O97252
E	177	HIS	-	cloning artifact	UNP O97252
E	178	MET	-	cloning artifact	UNP O97252
F	156	MET	-	cloning artifact	UNP O97252
F	157	GLY	-	cloning artifact	UNP O97252
F	158	SER	-	cloning artifact	UNP O97252
F	159	SER	-	cloning artifact	UNP O97252
F	160	HIS	-	expression tag	UNP O97252
F	161	HIS	-	expression tag	UNP O97252
F	162	HIS	-	expression tag	UNP O97252
F	163	HIS	-	expression tag	UNP O97252
F	164	HIS	-	expression tag	UNP O97252
F	165	HIS	-	expression tag	UNP O97252
F	166	SER	-	cloning artifact	UNP O97252
F	167	SER	-	cloning artifact	UNP O97252
F	168	GLY	-	cloning artifact	UNP O97252
F	169	ARG	-	cloning artifact	UNP O97252
F	170	GLU	-	cloning artifact	UNP O97252
F	171	ASN	-	cloning artifact	UNP O97252
F	172	LEU	-	cloning artifact	UNP O97252
F	173	TYR	-	cloning artifact	UNP O97252
F	174	PHE	-	cloning artifact	UNP O97252
F	175	GLN	-	cloning artifact	UNP O97252
F	176	GLY	-	cloning artifact	UNP O97252
F	177	HIS	-	cloning artifact	UNP O97252
F	178	MET	-	cloning artifact	UNP O97252
G	156	MET	-	cloning artifact	UNP O97252
G	157	GLY	-	cloning artifact	UNP O97252
G	158	SER	-	cloning artifact	UNP O97252

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Chain	Residue	Modelled	Actual	Comment	Reference
G	159	SER	-	cloning artifact	UNP O97252
G	160	HIS	-	expression tag	UNP O97252
G	161	HIS	-	expression tag	UNP O97252
G	162	HIS	-	expression tag	UNP O97252
G	163	HIS	-	expression tag	UNP O97252
G	164	HIS	-	expression tag	UNP O97252
G	165	HIS	-	expression tag	UNP O97252
G	166	SER	-	cloning artifact	UNP O97252
G	167	SER	-	cloning artifact	UNP O97252
G	168	GLY	-	cloning artifact	UNP O97252
G	169	ARG	-	cloning artifact	UNP O97252
G	170	GLU	-	cloning artifact	UNP O97252
G	171	ASN	-	cloning artifact	UNP O97252
G	172	LEU	-	cloning artifact	UNP O97252
G	173	TYR	-	cloning artifact	UNP O97252
G	174	PHE	-	cloning artifact	UNP O97252
G	175	GLN	-	cloning artifact	UNP O97252
G	176	GLY	-	cloning artifact	UNP O97252
G	177	HIS	-	cloning artifact	UNP O97252
G	178	MET	-	cloning artifact	UNP O97252

- Molecule 2 is water.

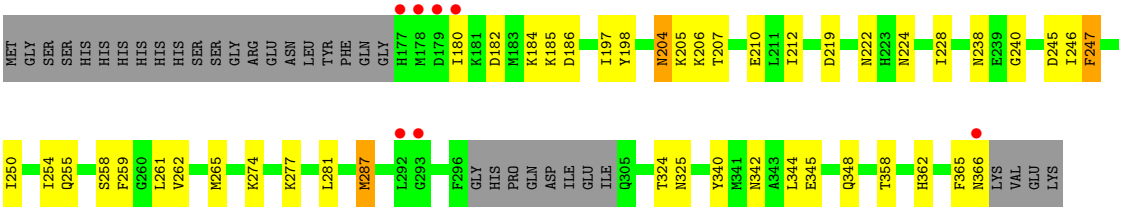
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O			
2	A	55	55	55		0	0
			Total	O			
2	B	41	41	41		0	0
			Total	O			
2	C	33	33	33		0	0
			Total	O			
2	D	23	23	23		0	0
			Total	O			
2	E	27	27	27		0	0
			Total	O			
2	F	35	35	35		0	0
			Total	O			
2	G	34	34	34		0	0

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.

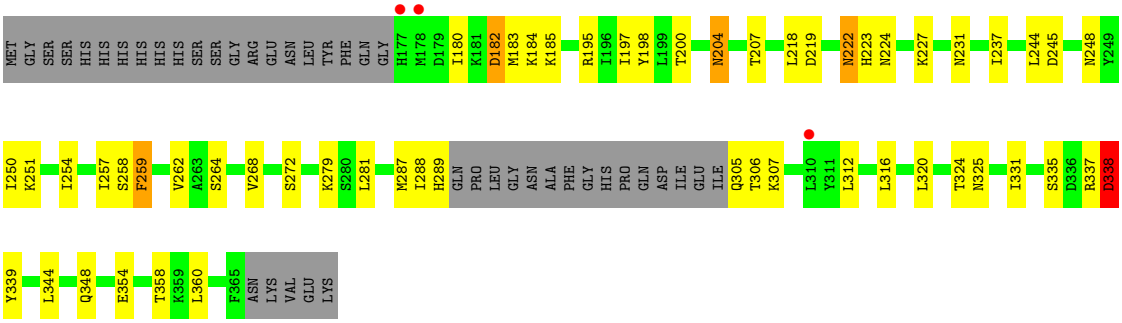
• Molecule 1: ATP-dependent CLP protease, putative

Chain A:



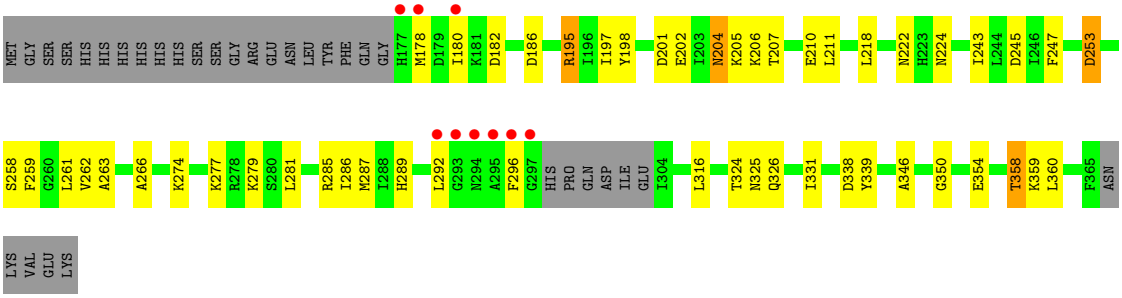
• Molecule 1: ATP-dependent CLP protease, putative

Chain B:



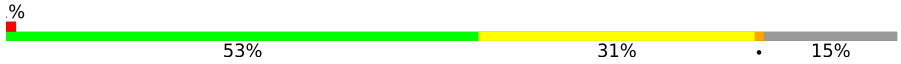
• Molecule 1: ATP-dependent CLP protease, putative

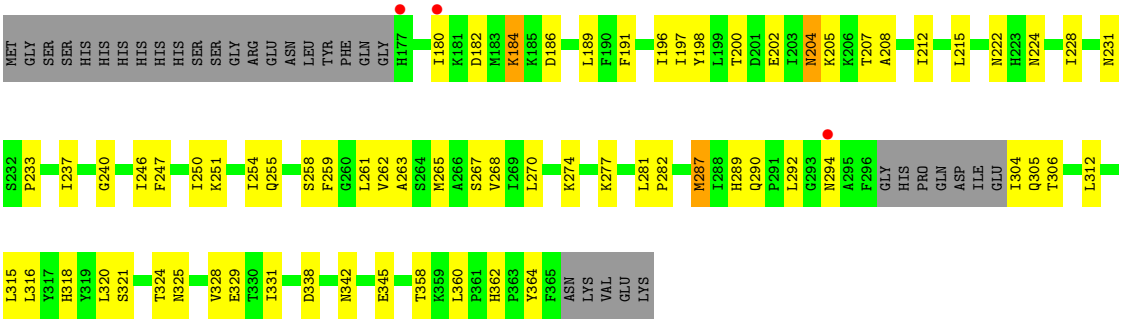
Chain C:



• Molecule 1: ATP-dependent CLP protease, putative

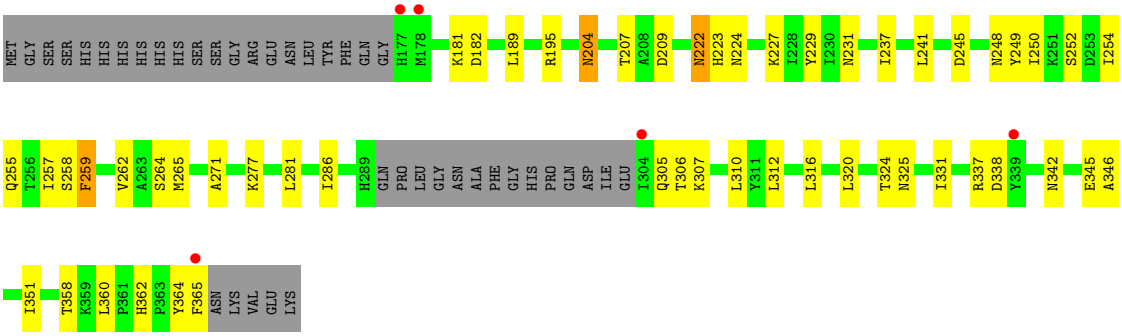
Chain D:





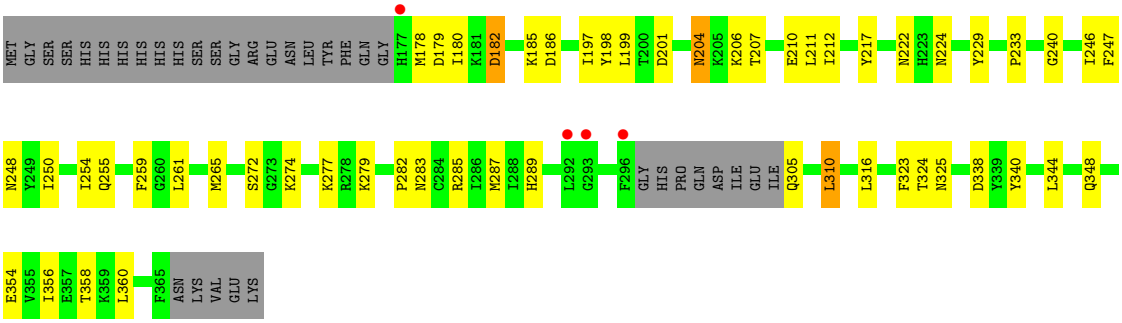
• Molecule 1: ATP-dependent CLP protease, putative

Chain E:



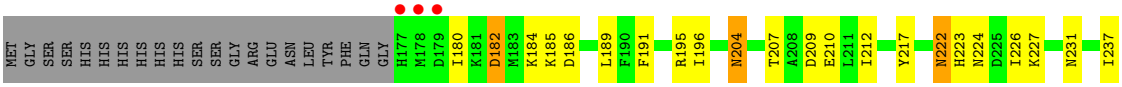
• Molecule 1: ATP-dependent CLP protease, putative

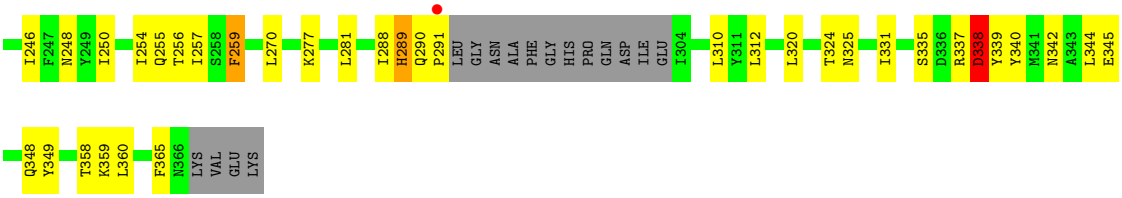
Chain F:



• Molecule 1: ATP-dependent CLP protease, putative

Chain G:




I246
F247
N248
Y249
I250
I254
Q255
T256
I257
S258
F259
L270
K277
L281
I288
H289
Q290
P291
LEU
GLY
ASN
ALA
PHE
GLY
HIS
PRO
GLN
ASP
ILE
GLU
I304
L310
Y311
L312
L320
T324
N325
I331
S335
D336
R337
D338
Y339
Y340
M341
N342
A343
L344
E345
Q348
Y349
T358
K359
L360
F365
N366
LYS
VAL
GLU
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	158.30Å 196.46Å 139.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.45 47.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.45) 96.3 (47.85-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.16 (at 2.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.238 0.210 , 0.238	Depositor DCC
R_{free} test set	3911 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10189	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.29	0/1472	0.53	0/1985
1	B	0.29	0/1411	0.54	0/1904
1	C	0.29	0/1476	0.52	0/1992
1	D	0.28	0/1459	0.50	0/1971
1	E	0.28	0/1415	0.52	0/1910
1	F	0.29	0/1459	0.53	0/1970
1	G	0.30	0/1422	0.56	1/1922 (0.1%)
All	All	0.29	0/10114	0.53	1/13654 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	291	PRO	N-CA-CB	5.75	110.20	103.30

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	1447	0	1452	37	0
1	B	1387	0	1386	49	0
1	C	1450	0	1447	50	0
1	D	1434	0	1426	56	0
1	E	1391	0	1386	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1434	0	1430	53	0
1	G	1398	0	1376	57	1
2	A	55	0	0	4	0
2	B	41	0	0	6	0
2	C	33	0	0	3	0
2	D	23	0	0	8	0
2	E	27	0	0	3	0
2	F	35	0	0	7	0
2	G	34	0	0	4	0
All	All	10189	0	9903	330	1

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 17.

All (330) 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:C:358:THR:HG22	1:C:360:LEU:H	1.20	1.02
1:D:240:GLY:HA3	1:D:265:MET:HG2	1.41	1.02
1:G:212:ILE:HB	2:G:402:HOH:O	1.59	1.01
1:G:358:THR:HG22	1:G:360:LEU:H	1.31	0.94
1:C:222:ASN:HD22	1:C:224:ASN:H	1.14	0.93
1:F:222:ASN:HD22	1:F:224:ASN:H	1.13	0.92
1:D:222:ASN:HD22	1:D:224:ASN:H	1.17	0.91
1:C:261:LEU:HD11	1:C:287:MET:HE1	1.50	0.91
1:A:222:ASN:HD22	1:A:224:ASN:H	1.16	0.88
1:F:261:LEU:HD11	1:F:287:MET:HE1	1.58	0.85
1:B:222:ASN:HD22	1:B:224:ASN:H	1.25	0.85
1:B:358:THR:HB	2:B:405:HOH:O	1.77	0.85
1:F:240:GLY:HA3	1:F:265:MET:HG2	1.57	0.84
1:D:222:ASN:ND2	1:D:224:ASN:H	1.77	0.82
1:F:204:ASN:ND2	1:F:207:THR:H	1.78	0.81
1:E:222:ASN:ND2	1:E:224:ASN:H	1.81	0.79
1:B:204:ASN:ND2	1:B:207:THR:H	1.80	0.78
1:B:222:ASN:ND2	1:B:224:ASN:H	1.82	0.78
1:D:250:ILE:HD11	1:D:254:ILE:HD11	1.66	0.77
1:G:259:PHE:HB3	1:G:281:LEU:HD12	1.67	0.77
1:A:204:ASN:ND2	1:A:207:THR:H	1.83	0.77
1:F:250:ILE:HD11	1:F:254:ILE:HD11	1.67	0.76
1:F:261:LEU:HD12	1:F:285:ARG:HB2	1.68	0.76
1:A:204:ASN:C	1:A:204:ASN:HD22	1.89	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:ASN:C	1:E:222:ASN:HD22	1.89	0.75
1:C:358:THR:CG2	1:C:360:LEU:H	1.98	0.74
1:C:222:ASN:ND2	1:C:224:ASN:H	1.84	0.74
1:G:365:PHE:HA	2:G:401:HOH:O	1.87	0.74
1:F:201:ASP:HB3	2:F:404:HOH:O	1.88	0.74
1:G:222:ASN:ND2	1:G:224:ASN:H	1.84	0.74
1:A:222:ASN:ND2	1:A:224:ASN:H	1.86	0.73
1:D:204:ASN:ND2	1:D:207:THR:H	1.87	0.72
1:C:204:ASN:HD22	1:C:204:ASN:C	1.91	0.72
1:G:342:ASN:HB2	1:G:365:PHE:HZ	1.54	0.72
1:F:222:ASN:ND2	1:F:224:ASN:H	1.86	0.71
1:A:204:ASN:HD21	1:A:207:THR:H	1.38	0.71
1:G:204:ASN:ND2	1:G:207:THR:H	1.88	0.71
1:E:204:ASN:ND2	1:E:207:THR:H	1.88	0.71
1:C:202:GLU:HG2	1:C:292:LEU:HD11	1.73	0.70
1:A:259:PHE:HB3	1:A:281:LEU:HD12	1.71	0.70
1:E:305:GLN:HE22	1:F:338:ASP:HB3	1.57	0.70
1:B:288:ILE:O	1:B:289:HIS:HB2	1.91	0.70
1:D:318:HIS:HB2	2:D:386:HOH:O	1.91	0.70
1:D:212:ILE:HG23	1:D:246:ILE:HG13	1.73	0.69
1:B:248:ASN:HB3	1:C:358:THR:HG23	1.72	0.69
1:C:358:THR:HG22	1:C:360:LEU:N	2.02	0.69
1:D:328:VAL:HG22	2:D:390:HOH:O	1.93	0.69
1:C:204:ASN:ND2	1:C:207:THR:H	1.91	0.68
1:B:358:THR:HG23	1:B:360:LEU:H	1.58	0.68
1:C:261:LEU:HD11	1:C:287:MET:CE	2.23	0.68
1:D:204:ASN:C	1:D:204:ASN:HD22	1.97	0.68
1:E:365:PHE:HA	2:E:381:HOH:O	1.93	0.68
1:C:253:ASP:OD2	1:C:274:LYS:HE2	1.92	0.68
1:E:204:ASN:HD22	1:E:204:ASN:C	1.97	0.67
1:G:259:PHE:CB	1:G:281:LEU:HD12	2.26	0.65
1:A:255:GLN:HG2	1:A:277:LYS:HB3	1.78	0.65
1:F:204:ASN:C	1:F:204:ASN:HD22	2.00	0.65
1:E:195:ARG:NH1	1:E:224:ASN:O	2.30	0.64
1:F:274:LYS:HB3	1:F:277:LYS:HD2	1.78	0.64
1:G:358:THR:HG22	1:G:360:LEU:N	2.08	0.64
1:E:358:THR:HG23	1:E:360:LEU:H	1.63	0.64
1:G:222:ASN:HD22	1:G:224:ASN:H	1.45	0.64
1:B:195:ARG:NH2	1:B:218:LEU:O	2.30	0.64
1:B:204:ASN:HD21	1:B:207:THR:H	1.42	0.64
1:C:204:ASN:HD21	1:C:207:THR:H	1.43	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:TYR:HB3	2:C:379:HOH:O	1.98	0.64
1:E:250:ILE:HD11	1:E:254:ILE:HD11	1.81	0.63
1:D:265:MET:HB2	2:D:371:HOH:O	1.99	0.63
1:F:240:GLY:HA3	1:F:265:MET:CG	2.26	0.63
1:B:204:ASN:C	1:B:204:ASN:HD22	2.02	0.62
1:C:253:ASP:HB3	1:C:274:LYS:HE2	1.81	0.62
1:G:222:ASN:HD22	1:G:222:ASN:C	2.02	0.62
1:D:289:HIS:CD2	1:D:338:ASP:HA	2.34	0.62
1:A:206:LYS:O	1:A:210:GLU:HG3	1.99	0.62
1:C:325:ASN:HB3	2:C:396:HOH:O	1.99	0.62
1:F:204:ASN:HD21	1:F:207:THR:H	1.48	0.62
1:C:253:ASP:CB	1:C:274:LYS:HE2	2.31	0.61
1:A:324:THR:O	1:A:325:ASN:HB2	2.00	0.61
1:E:305:GLN:NE2	1:F:338:ASP:HB3	2.15	0.61
1:D:324:THR:O	1:D:325:ASN:HB2	2.01	0.60
1:B:306:THR:HG23	1:B:307:LYS:N	2.16	0.60
2:D:373:HOH:O	1:E:358:THR:HG21	2.00	0.60
1:F:255:GLN:HB3	1:F:277:LYS:HB3	1.83	0.60
1:G:342:ASN:HB2	1:G:365:PHE:CZ	2.36	0.60
1:E:255:GLN:HB3	1:E:277:LYS:HB3	1.83	0.60
1:E:227:LYS:HD3	1:E:257:ILE:HD12	1.84	0.59
1:G:195:ARG:HH12	1:G:226:ILE:HG13	1.67	0.59
1:G:204:ASN:C	1:G:204:ASN:HD22	2.06	0.59
1:F:305:GLN:HG2	1:G:340:TYR:HE1	1.68	0.59
1:D:320:LEU:HD23	1:D:331:ILE:HG23	1.85	0.59
1:A:182:ASP:OD2	1:A:185:LYS:N	2.36	0.58
1:C:245:ASP:HB3	1:D:281:LEU:HD13	1.84	0.58
1:D:263:ALA:HB2	1:D:287:MET:SD	2.44	0.58
1:D:240:GLY:HA3	1:D:265:MET:CG	2.26	0.57
1:E:222:ASN:HD22	1:E:223:HIS:N	2.01	0.57
1:B:289:HIS:ND1	1:B:335:SER:O	2.38	0.57
1:C:195:ARG:NH2	1:C:218:LEU:O	2.36	0.57
1:B:248:ASN:CB	1:C:358:THR:HG23	2.34	0.57
1:F:344:LEU:O	1:F:348:GLN:HG3	2.04	0.57
1:C:258:SER:HB2	1:C:262:VAL:HG21	1.87	0.57
1:F:282:PRO:HG2	1:F:358:THR:HG22	1.85	0.57
1:D:342:ASN:OD1	1:D:345:GLU:HG3	2.03	0.57
1:G:209:ASP:C	2:G:402:HOH:O	2.43	0.56
1:E:222:ASN:ND2	1:E:222:ASN:C	2.59	0.56
1:B:259:PHE:HB3	1:B:281:LEU:HD12	1.86	0.56
2:B:408:HOH:O	1:C:358:THR:HG21	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:THR:HG23	1:E:307:LYS:N	2.21	0.56
1:F:182:ASP:OD1	1:F:185:LYS:N	2.39	0.56
1:C:206:LYS:O	1:C:210:GLU:HG3	2.06	0.55
2:A:383:HOH:O	1:B:358:THR:HG21	2.07	0.55
1:F:282:PRO:HG2	1:F:358:THR:CG2	2.36	0.55
1:G:320:LEU:HD23	1:G:331:ILE:HG23	1.88	0.55
1:B:183:MET:HA	2:B:407:HOH:O	2.07	0.55
1:D:222:ASN:HD22	1:D:224:ASN:N	1.97	0.55
1:A:184:LYS:HE2	1:G:210:GLU:OE1	2.08	0.54
1:C:259:PHE:HB3	1:C:281:LEU:HD12	1.89	0.54
1:E:241:LEU:HD21	2:E:395:HOH:O	2.06	0.54
1:G:195:ARG:HH12	1:G:226:ILE:CG1	2.19	0.54
1:C:180:ILE:HG12	1:C:186:ASP:HB3	1.88	0.54
1:B:268:VAL:HG21	1:B:316:LEU:HD21	1.89	0.54
1:B:324:THR:O	1:B:325:ASN:HB2	2.07	0.53
1:A:274:LYS:HB3	1:A:277:LYS:HD2	1.91	0.53
1:E:237:ILE:HG21	1:E:312:LEU:HB3	1.90	0.53
1:F:324:THR:O	1:F:325:ASN:HB2	2.07	0.53
1:C:211:LEU:HD23	1:C:243:ILE:HD13	1.89	0.53
1:G:204:ASN:HD21	1:G:207:THR:H	1.56	0.53
1:G:342:ASN:OD1	1:G:345:GLU:HG3	2.09	0.53
1:E:305:GLN:NE2	1:F:340:TYR:HE1	2.07	0.53
1:B:258:SER:HB2	1:B:262:VAL:HG21	1.91	0.52
1:D:180:ILE:HG23	1:D:186:ASP:HB2	1.90	0.52
1:B:223:HIS:CD2	1:B:251:LYS:HB2	2.44	0.52
2:E:389:HOH:O	1:F:283:ASN:N	2.42	0.52
1:D:205:LYS:NZ	2:D:387:HOH:O	2.42	0.52
1:D:255:GLN:HB3	1:D:277:LYS:HB3	1.92	0.52
1:E:231:ASN:HB2	1:E:259:PHE:CE2	2.45	0.52
1:D:315:LEU:C	2:D:386:HOH:O	2.47	0.52
1:F:261:LEU:CD1	1:F:285:ARG:HB2	2.39	0.52
1:F:358:THR:HG23	1:F:360:LEU:O	2.10	0.52
1:G:195:ARG:NH1	1:G:226:ILE:HG12	2.24	0.52
1:A:212:ILE:HG23	1:A:246:ILE:HG13	1.91	0.51
1:D:251:LYS:HD2	1:D:251:LYS:N	2.25	0.51
1:G:209:ASP:O	2:G:402:HOH:O	2.18	0.51
1:F:316:LEU:HD23	1:F:316:LEU:C	2.31	0.51
1:G:222:ASN:HD22	1:G:223:HIS:N	2.09	0.51
1:D:237:ILE:HG21	1:D:312:LEU:HB3	1.91	0.51
1:G:337:ARG:O	1:G:338:ASP:C	2.49	0.51
1:E:362:HIS:HB3	1:E:365:PHE:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:THR:HG22	2:B:381:HOH:O	2.10	0.50
1:C:204:ASN:C	1:C:204:ASN:ND2	2.64	0.50
1:C:274:LYS:HD2	1:C:277:LYS:HD2	1.93	0.50
1:C:326:GLN:HB2	1:C:331:ILE:HD11	1.93	0.50
1:E:337:ARG:O	1:E:338:ASP:C	2.50	0.50
1:B:195:ARG:NH1	1:B:224:ASN:O	2.45	0.50
1:B:259:PHE:CB	1:B:281:LEU:HD12	2.41	0.50
1:C:324:THR:O	1:C:325:ASN:HB2	2.11	0.50
1:E:245:ASP:OD2	1:F:283:ASN:HB2	2.12	0.50
1:G:255:GLN:HB3	1:G:277:LYS:HB3	1.92	0.50
1:C:253:ASP:HB3	1:C:274:LYS:CE	2.41	0.50
1:F:261:LEU:HD11	1:F:287:MET:CE	2.38	0.50
1:D:233:PRO:HG2	1:D:292:LEU:HD11	1.93	0.49
1:E:204:ASN:HD21	1:E:207:THR:H	1.58	0.49
1:F:272:SER:HB3	1:F:323:PHE:CE1	2.47	0.49
1:E:306:THR:HG23	1:E:307:LYS:H	1.77	0.49
1:F:229:TYR:HB3	1:F:259:PHE:HE1	1.77	0.49
1:F:233:PRO:HA	2:F:400:HOH:O	2.11	0.49
1:F:279:LYS:HG2	1:F:354:GLU:HG2	1.93	0.49
1:A:247:PHE:CE2	1:A:254:ILE:HG21	2.46	0.49
1:F:265:MET:HB2	2:F:371:HOH:O	2.12	0.49
1:B:344:LEU:O	1:B:348:GLN:HG3	2.13	0.49
1:D:261:LEU:HD11	1:D:287:MET:SD	2.52	0.49
1:E:259:PHE:C	1:E:259:PHE:CD2	2.85	0.49
1:A:180:ILE:HG23	1:A:182:ASP:O	2.12	0.49
1:B:264:SER:HB2	1:B:289:HIS:O	2.13	0.49
1:E:259:PHE:CB	1:E:281:LEU:HD12	2.43	0.49
1:A:204:ASN:ND2	1:A:204:ASN:C	2.62	0.49
1:E:189:LEU:HD11	1:F:180:ILE:HG22	1.93	0.49
1:G:182:ASP:O	1:G:186:ASP:HB2	2.11	0.49
1:A:358:THR:HB	1:G:248:ASN:O	2.13	0.49
1:G:195:ARG:NH1	1:G:226:ILE:CG1	2.76	0.49
1:D:318:HIS:CB	2:D:386:HOH:O	2.58	0.48
1:G:195:ARG:NH1	1:G:224:ASN:O	2.46	0.48
1:A:344:LEU:O	1:A:348:GLN:HG3	2.13	0.48
1:B:183:MET:HG3	2:B:407:HOH:O	2.13	0.48
1:E:222:ASN:HD22	1:E:224:ASN:H	1.55	0.48
1:G:180:ILE:HG23	1:G:182:ASP:O	2.13	0.48
1:D:282:PRO:HG2	1:D:358:THR:HG22	1.96	0.48
1:D:358:THR:HG23	1:D:360:LEU:O	2.13	0.48
1:A:342:ASN:OD1	1:A:345:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:SER:HB2	1:E:262:VAL:HG21	1.95	0.48
1:G:358:THR:CG2	1:G:359:LYS:N	2.77	0.48
1:G:222:ASN:ND2	1:G:222:ASN:C	2.67	0.48
1:F:261:LEU:HG	2:F:400:HOH:O	2.13	0.48
1:C:274:LYS:NZ	1:C:277:LYS:NZ	2.62	0.47
1:E:259:PHE:C	1:E:259:PHE:HD2	2.18	0.47
1:G:289:HIS:ND1	1:G:335:SER:O	2.42	0.47
1:B:320:LEU:HD23	1:B:331:ILE:HG23	1.96	0.47
1:D:202:GLU:OE2	1:D:292:LEU:HD13	2.14	0.47
1:D:318:HIS:N	2:D:386:HOH:O	2.40	0.47
1:D:180:ILE:HG23	1:D:186:ASP:CB	2.45	0.47
1:D:191:PHE:HB3	1:D:196:ILE:HB	1.95	0.47
1:A:261:LEU:HD23	1:A:262:VAL:N	2.30	0.47
1:E:259:PHE:HB3	1:E:281:LEU:HD12	1.96	0.47
1:F:199:LEU:HD13	1:F:211:LEU:HD22	1.96	0.47
1:A:240:GLY:HA3	1:A:265:MET:HG3	1.97	0.47
1:C:253:ASP:CG	1:C:274:LYS:HE2	2.34	0.47
2:C:399:HOH:O	1:D:180:ILE:HB	2.15	0.47
1:D:258:SER:HB2	1:D:262:VAL:HG21	1.97	0.47
2:A:392:HOH:O	1:B:183:MET:HE2	2.15	0.47
1:F:305:GLN:HG2	1:G:340:TYR:CE1	2.50	0.47
1:G:237:ILE:HG21	1:G:312:LEU:HB3	1.97	0.47
1:B:337:ARG:O	1:B:338:ASP:C	2.53	0.46
1:E:320:LEU:HD23	1:E:331:ILE:HG23	1.97	0.46
1:E:209:ASP:HB2	2:F:399:HOH:O	2.14	0.46
1:B:204:ASN:ND2	1:B:204:ASN:C	2.68	0.46
1:G:344:LEU:O	1:G:348:GLN:HG3	2.15	0.46
1:D:215:LEU:HD21	1:D:228:ILE:HD11	1.97	0.46
1:G:365:PHE:N	1:G:365:PHE:CD2	2.84	0.46
1:D:197:ILE:HG22	1:D:198:TYR:N	2.31	0.46
1:E:271:ALA:HB2	1:E:351:ILE:HG23	1.98	0.46
1:G:182:ASP:OD1	1:G:185:LYS:N	2.49	0.45
1:A:228:ILE:HD12	1:A:247:PHE:CZ	2.51	0.45
1:B:245:ASP:HB3	1:C:281:LEU:HD13	1.98	0.45
1:G:250:ILE:HD11	1:G:254:ILE:HD11	1.98	0.45
1:C:261:LEU:HD12	1:C:285:ARG:O	2.16	0.45
1:F:197:ILE:HG22	1:F:198:TYR:N	2.32	0.45
1:G:231:ASN:HB2	1:G:259:PHE:CE2	2.52	0.45
1:D:259:PHE:HB3	1:D:281:LEU:HD12	1.98	0.45
1:B:244:LEU:HD11	1:B:272:SER:CB	2.46	0.45
1:D:204:ASN:HD22	1:D:207:THR:H	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ALA:O	1:C:266:ALA:HB3	2.17	0.45
1:E:342:ASN:ND2	1:E:345:GLU:HG3	2.32	0.45
1:F:212:ILE:HG23	1:F:246:ILE:HG13	1.99	0.45
1:B:180:ILE:O	1:B:180:ILE:HG13	2.17	0.45
1:B:182:ASP:OD1	1:B:184:LYS:N	2.46	0.44
1:F:289:HIS:HD2	2:F:393:HOH:O	2.00	0.44
1:B:306:THR:CG2	1:B:307:LYS:N	2.80	0.44
1:G:227:LYS:HD3	1:G:257:ILE:HD12	1.99	0.44
1:A:180:ILE:HD12	1:G:217:TYR:CZ	2.53	0.44
1:A:258:SER:HB2	1:A:262:VAL:HG21	1.99	0.44
1:D:184:LYS:HD2	1:D:184:LYS:N	2.32	0.44
1:F:204:ASN:HD22	1:F:207:THR:H	1.60	0.44
1:G:182:ASP:OD1	1:G:184:LYS:N	2.45	0.44
1:A:365:PHE:HB3	1:A:366:ASN:H	1.62	0.44
1:B:222:ASN:HD22	1:B:222:ASN:C	2.21	0.44
1:C:289:HIS:CD2	1:C:338:ASP:HA	2.53	0.44
1:D:189:LEU:HD22	1:E:181:LYS:O	2.18	0.44
1:D:274:LYS:HB3	1:D:277:LYS:HD2	1.99	0.44
1:G:358:THR:HG22	1:G:359:LYS:N	2.33	0.44
1:A:238:ASN:HB3	2:A:386:HOH:O	2.17	0.44
1:A:259:PHE:CB	1:A:281:LEU:HD12	2.44	0.44
1:B:279:LYS:HG2	1:B:354:GLU:HG2	2.00	0.44
1:B:250:ILE:HD11	1:B:254:ILE:HD11	2.00	0.44
1:G:342:ASN:CG	1:G:345:GLU:HG3	2.38	0.44
1:E:249:TYR:CE2	1:F:356:ILE:HG21	2.52	0.43
1:E:316:LEU:C	1:E:316:LEU:HD23	2.37	0.43
1:C:259:PHE:CB	1:C:281:LEU:HD12	2.48	0.43
1:D:200:THR:HA	1:D:231:ASN:O	2.18	0.43
1:A:287:MET:HE3	1:A:340:TYR:CZ	2.54	0.43
1:B:279:LYS:HE2	1:B:354:GLU:CD	2.39	0.43
1:D:290:GLN:NE2	1:D:294:ASN:HA	2.34	0.43
1:F:206:LYS:O	1:F:210:GLU:HG3	2.19	0.43
1:F:289:HIS:CD2	1:F:338:ASP:HA	2.53	0.43
1:B:305:GLN:HE22	1:C:338:ASP:CB	2.31	0.43
1:E:316:LEU:HD23	1:E:316:LEU:O	2.18	0.43
1:C:279:LYS:HE2	1:C:354:GLU:OE2	2.19	0.43
1:B:219:ASP:OD1	1:B:223:HIS:HD2	2.02	0.43
1:F:182:ASP:O	1:F:186:ASP:HB2	2.19	0.43
1:G:259:PHE:CD2	1:G:259:PHE:C	2.92	0.43
1:B:306:THR:HG23	1:B:307:LYS:H	1.83	0.43
1:C:197:ILE:HG22	1:C:198:TYR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:MET:HE3	1:D:268:VAL:HB	2.01	0.43
1:D:316:LEU:HD23	1:D:316:LEU:C	2.39	0.43
1:E:286:ILE:HD12	1:E:346:ALA:CB	2.49	0.43
1:C:324:THR:HG22	1:C:350:GLY:O	2.19	0.42
1:D:282:PRO:HG2	1:D:358:THR:CG2	2.50	0.42
1:E:324:THR:O	1:E:325:ASN:HB2	2.18	0.42
1:G:191:PHE:HB3	1:G:196:ILE:HB	2.01	0.42
1:A:197:ILE:HG22	1:A:198:TYR:N	2.34	0.42
1:F:180:ILE:HG23	1:F:182:ASP:O	2.19	0.42
1:F:310:LEU:HD23	1:F:310:LEU:HA	1.92	0.42
1:B:237:ILE:HG21	1:B:312:LEU:HB3	2.01	0.42
1:G:212:ILE:HG23	1:G:246:ILE:HG13	2.02	0.42
1:B:182:ASP:OD1	1:B:185:LYS:N	2.53	0.42
1:F:305:GLN:N	2:F:402:HOH:O	2.51	0.42
1:D:208:ALA:O	1:D:212:ILE:HG13	2.19	0.42
1:E:362:HIS:HE1	1:E:364:TYR:CD2	2.38	0.42
1:G:324:THR:O	1:G:325:ASN:HB2	2.20	0.42
1:A:362:HIS:HB3	1:A:365:PHE:HB2	2.02	0.41
1:D:318:HIS:O	1:D:321:SER:HB3	2.20	0.41
1:E:204:ASN:ND2	1:E:204:ASN:C	2.69	0.41
1:E:265:MET:HE3	1:E:265:MET:O	2.20	0.41
1:G:288:ILE:HD11	1:G:349:TYR:CE2	2.55	0.41
1:B:200:THR:HA	1:B:231:ASN:O	2.20	0.41
1:C:286:ILE:HD12	1:C:346:ALA:CB	2.51	0.41
1:D:329:GLU:H	1:D:329:GLU:CD	2.23	0.41
1:F:248:ASN:HB3	1:G:358:THR:CG2	2.50	0.41
1:A:180:ILE:HG22	1:G:189:LEU:HD11	2.01	0.41
1:C:358:THR:CG2	1:C:359:LYS:N	2.83	0.41
1:E:342:ASN:OD1	1:E:345:GLU:HG3	2.20	0.41
1:G:256:THR:HB	1:G:270:LEU:HD12	2.01	0.41
1:A:245:ASP:HB3	1:B:281:LEU:HD13	2.01	0.41
1:B:287:MET:HE2	1:B:338:ASP:CA	2.50	0.41
1:C:274:LYS:HZ2	1:C:277:LYS:HZ1	1.68	0.41
1:D:304:ILE:O	1:D:306:THR:N	2.53	0.41
1:A:180:ILE:HG12	1:A:186:ASP:HB3	2.02	0.41
1:C:180:ILE:HG23	1:C:182:ASP:O	2.21	0.41
1:D:267:SER:O	1:D:270:LEU:HB3	2.21	0.41
1:F:204:ASN:ND2	1:F:204:ASN:C	2.72	0.41
1:A:205:LYS:NZ	2:A:389:HOH:O	2.52	0.41
1:F:217:TYR:CZ	1:G:180:ILE:HD12	2.56	0.41
1:A:219:ASP:CG	1:A:250:ILE:HB	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:LYS:HD3	1:B:257:ILE:HD12	2.03	0.41
1:E:342:ASN:CG	1:E:345:GLU:HG3	2.41	0.41
1:F:222:ASN:HD22	1:F:224:ASN:N	1.96	0.41
2:B:383:HOH:O	1:C:178:MET:HE1	2.21	0.41
1:E:264:SER:OG	1:E:265:MET:N	2.52	0.41
1:C:287:MET:HB2	1:C:289:HIS:CD2	2.56	0.40
1:C:316:LEU:C	1:C:316:LEU:HD23	2.41	0.40
1:E:229:TYR:HA	1:E:257:ILE:O	2.21	0.40
1:G:231:ASN:HD22	1:G:259:PHE:HE2	1.68	0.40
1:D:316:LEU:HD23	1:D:316:LEU:O	2.21	0.40
1:D:362:HIS:HE1	1:D:364:TYR:CD2	2.39	0.40
1:E:248:ASN:HB3	1:F:358:THR:OG1	2.21	0.40
1:A:180:ILE:CG2	1:A:182:ASP:O	2.70	0.40
1:B:197:ILE:HG22	1:B:198:TYR:N	2.37	0.40
1:E:223:HIS:HA	1:E:252:SER:OG	2.21	0.40
1:C:205:LYS:HE3	1:D:200:THR:O	2.22	0.40
1:G:195:ARG:NE	1:G:222:ASN:HD21	2.19	0.40
1:A:261:LEU:HD23	1:A:261:LEU:C	2.42	0.40
1:D:274:LYS:HG2	1:D:277:LYS:HD2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:310:LEU:CD1	1:G:310:LEU:CD1[3_555]	2.01	0.19

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	178/215 (83%)	171 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	170/215 (79%)	163 (96%)	6 (4%)	1 (1%)	25	29
1	C	179/215 (83%)	170 (95%)	8 (4%)	1 (1%)	25	29
1	D	178/215 (83%)	163 (92%)	14 (8%)	1 (1%)	25	29
1	E	171/215 (80%)	165 (96%)	6 (4%)	0	100	100
1	F	177/215 (82%)	165 (93%)	10 (6%)	2 (1%)	14	14
1	G	174/215 (81%)	164 (94%)	7 (4%)	3 (2%)	9	7
All	All	1227/1505 (82%)	1161 (95%)	58 (5%)	8 (1%)	22	25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	305	GLN
1	G	290	GLN
1	B	338	ASP
1	G	338	ASP
1	F	178	MET
1	C	296	PHE
1	F	179	ASP
1	G	289	HIS

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	157/195 (80%)	154 (98%)	3 (2%)	57	69
1	B	151/195 (77%)	145 (96%)	6 (4%)	31	41
1	C	157/195 (80%)	151 (96%)	6 (4%)	33	43
1	D	154/195 (79%)	149 (97%)	5 (3%)	39	50
1	E	151/195 (77%)	146 (97%)	5 (3%)	38	49
1	F	155/195 (80%)	151 (97%)	4 (3%)	46	58
1	G	149/195 (76%)	143 (96%)	6 (4%)	31	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1074/1365 (79%)	1039 (97%)	35 (3%)	38 49

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	A	247	PHE
1	A	287	MET
1	B	182	ASP
1	B	204	ASN
1	B	222	ASN
1	B	259	PHE
1	B	338	ASP
1	B	339	TYR
1	C	195	ARG
1	C	201	ASP
1	C	204	ASN
1	C	247	PHE
1	C	253	ASP
1	C	358	THR
1	D	182	ASP
1	D	184	LYS
1	D	204	ASN
1	D	247	PHE
1	D	287	MET
1	E	182	ASP
1	E	204	ASN
1	E	222	ASN
1	E	259	PHE
1	E	310	LEU
1	F	182	ASP
1	F	204	ASN
1	F	247	PHE
1	F	310	LEU
1	G	182	ASP
1	G	204	ASN
1	G	222	ASN
1	G	259	PHE
1	G	338	ASP
1	G	339	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	A	222	ASN
1	A	224	ASN
1	A	289	HIS
1	B	204	ASN
1	B	222	ASN
1	B	223	HIS
1	B	224	ASN
1	B	283	ASN
1	B	305	GLN
1	C	204	ASN
1	C	222	ASN
1	C	223	HIS
1	C	224	ASN
1	C	289	HIS
1	D	204	ASN
1	D	222	ASN
1	D	224	ASN
1	D	248	ASN
1	D	255	GLN
1	D	283	ASN
1	D	289	HIS
1	D	290	GLN
1	E	204	ASN
1	E	222	ASN
1	E	223	HIS
1	E	283	ASN
1	E	305	GLN
1	F	204	ASN
1	F	222	ASN
1	G	204	ASN
1	G	222	ASN
1	G	223	HIS

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)

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 (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	182/215 (84%)	-0.12	7 (3%)	40	37	34, 44, 69, 93	0
1	B	174/215 (80%)	-0.15	3 (1%)	70	67	32, 45, 70, 92	0
1	C	183/215 (85%)	-0.02	9 (4%)	29	27	41, 53, 74, 89	0
1	D	182/215 (84%)	0.06	3 (1%)	72	69	45, 57, 73, 88	0
1	E	175/215 (81%)	0.00	5 (2%)	51	47	38, 50, 76, 93	0
1	F	181/215 (84%)	-0.19	4 (2%)	62	58	34, 47, 72, 89	0
1	G	178/215 (82%)	-0.09	4 (2%)	62	58	32, 43, 72, 97	0
All	All	1255/1505 (83%)	-0.07	35 (2%)	53	49	32, 50, 74, 97	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	177	HIS	4.9
1	A	177	HIS	4.5
1	C	295	ALA	4.5
1	B	178	MET	4.1
1	E	177	HIS	3.7
1	C	178	MET	3.5
1	G	178	MET	3.4
1	A	179	ASP	3.4
1	C	296	PHE	3.3
1	E	178	MET	3.2
1	C	297	GLY	3.2
1	A	178	MET	2.9
1	B	177	HIS	2.9
1	A	293	GLY	2.8
1	F	293	GLY	2.8
1	A	366	ASN	2.8
1	C	292	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	291	PRO	2.6
1	E	304	ILE	2.6
1	D	177	HIS	2.6
1	D	294	ASN	2.6
1	F	292	LEU	2.5
1	B	310	LEU	2.5
1	D	180	ILE	2.4
1	C	294	ASN	2.4
1	F	296	PHE	2.4
1	A	292	LEU	2.4
1	G	179	ASP	2.3
1	C	177	HIS	2.3
1	F	177	HIS	2.2
1	A	180	ILE	2.1
1	C	293	GLY	2.1
1	E	339	TYR	2.1
1	E	365	PHE	2.1
1	C	180	ILE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.