Full wwPDB X-ray Structure Validation Report

Feb 19, 2016 – 06:38 PM GMT

PDB ID	:	3WUU
Title	:	Structure basis of inactivating cell abscission with chimera peptide 1
Authors	:	Kim, H.J.; Matsuura, A.; Lee, H.H.
Deposited on	:	2014-05-05
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

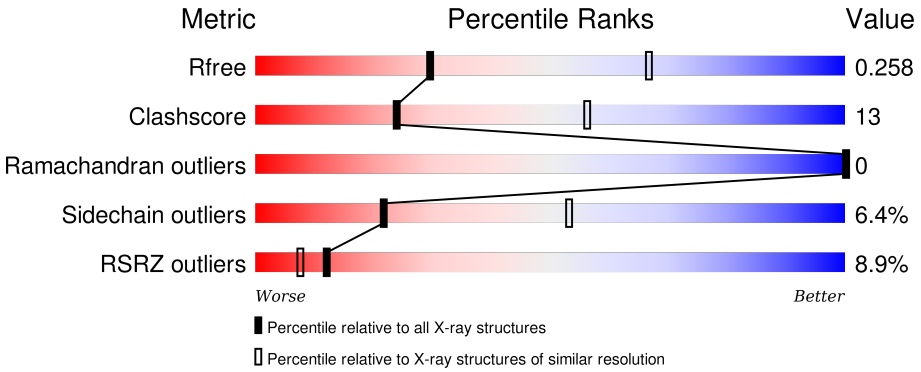
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	63	6% 83% • • 14%
1	B	63	3% 71% 6% • 21%
1	D	63	6% 57% 11% • 30%
1	E	63	5% 37% 22% 8% • 30%
1	G	63	5% 51% 21% • 27%

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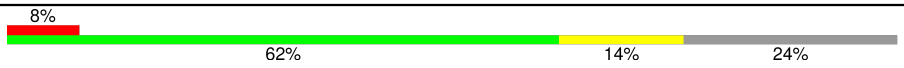
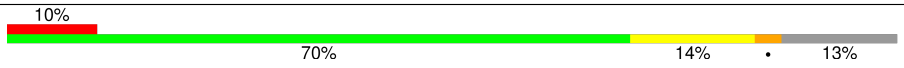
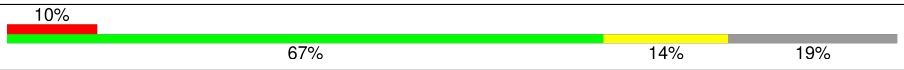
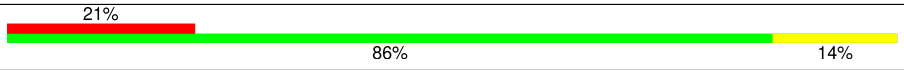
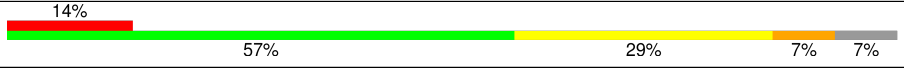
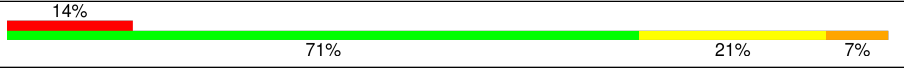
Mol	Chain	Length	Quality of chain
1	H	63	
1	J	63	
1	K	63	
2	C	14	
2	F	14	
2	I	14	
2	L	14	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3787 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 Centrosomal protein of 55 kDa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	54	Total	C	N	O	S	0	0	0
			447	285	75	85	2			
1	B	50	Total	C	N	O	S	0	0	0
			423	271	71	80	1			
1	D	44	Total	C	N	O	S	0	0	0
			377	242	62	72	1			
1	E	44	Total	C	N	O	S	0	0	0
			377	242	62	72	1			
1	G	46	Total	C	N	O	S	0	0	0
			394	252	66	75	1			
1	H	48	Total	C	N	O	S	0	0	0
			405	259	68	77	1			
1	J	55	Total	C	N	O	S	0	0	0
			456	290	76	88	2			
1	K	51	Total	C	N	O	S	0	0	0
			430	275	72	82	1			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	GLY	-	EXPRESSION TAG	UNP Q53EZ4
A	156	ALA	-	EXPRESSION TAG	UNP Q53EZ4
A	157	MET	-	EXPRESSION TAG	UNP Q53EZ4
A	158	GLY	-	EXPRESSION TAG	UNP Q53EZ4
A	159	SER	-	EXPRESSION TAG	UNP Q53EZ4
B	155	GLY	-	EXPRESSION TAG	UNP Q53EZ4
B	156	ALA	-	EXPRESSION TAG	UNP Q53EZ4
B	157	MET	-	EXPRESSION TAG	UNP Q53EZ4
B	158	GLY	-	EXPRESSION TAG	UNP Q53EZ4
B	159	SER	-	EXPRESSION TAG	UNP Q53EZ4
D	155	GLY	-	EXPRESSION TAG	UNP Q53EZ4
D	156	ALA	-	EXPRESSION TAG	UNP Q53EZ4
D	157	MET	-	EXPRESSION TAG	UNP Q53EZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	158	GLY	-	EXPRESSION TAG	UNP Q53EZ4
D	159	SER	-	EXPRESSION TAG	UNP Q53EZ4
E	155	GLY	-	EXPRESSION TAG	UNP Q53EZ4
E	156	ALA	-	EXPRESSION TAG	UNP Q53EZ4
E	157	MET	-	EXPRESSION TAG	UNP Q53EZ4
E	158	GLY	-	EXPRESSION TAG	UNP Q53EZ4
E	159	SER	-	EXPRESSION TAG	UNP Q53EZ4
G	155	GLY	-	EXPRESSION TAG	UNP Q53EZ4
G	156	ALA	-	EXPRESSION TAG	UNP Q53EZ4
G	157	MET	-	EXPRESSION TAG	UNP Q53EZ4
G	158	GLY	-	EXPRESSION TAG	UNP Q53EZ4
G	159	SER	-	EXPRESSION TAG	UNP Q53EZ4
H	155	GLY	-	EXPRESSION TAG	UNP Q53EZ4
H	156	ALA	-	EXPRESSION TAG	UNP Q53EZ4
H	157	MET	-	EXPRESSION TAG	UNP Q53EZ4
H	158	GLY	-	EXPRESSION TAG	UNP Q53EZ4
H	159	SER	-	EXPRESSION TAG	UNP Q53EZ4
J	155	GLY	-	EXPRESSION TAG	UNP Q53EZ4
J	156	ALA	-	EXPRESSION TAG	UNP Q53EZ4
J	157	MET	-	EXPRESSION TAG	UNP Q53EZ4
J	158	GLY	-	EXPRESSION TAG	UNP Q53EZ4
J	159	SER	-	EXPRESSION TAG	UNP Q53EZ4
K	155	GLY	-	EXPRESSION TAG	UNP Q53EZ4
K	156	ALA	-	EXPRESSION TAG	UNP Q53EZ4
K	157	MET	-	EXPRESSION TAG	UNP Q53EZ4
K	158	GLY	-	EXPRESSION TAG	UNP Q53EZ4
K	159	SER	-	EXPRESSION TAG	UNP Q53EZ4

- Molecule 2 is a protein called TEX-14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	0	0	0
			103	68	15	20			
2	F	13	Total	C	N	O	0	0	0
			95	64	14	17			
2	I	14	Total	C	N	O	0	0	0
			103	68	15	20			
2	L	14	Total	C	N	O	0	0	0
			103	68	15	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	791	ASP	PRO	ENGINEERED MUTATION	UNP Q8IWB6
C	802	PRO	ILE	ENGINEERED MUTATION	UNP Q8IWB6
C	803	GLY	PRO	ENGINEERED MUTATION	UNP Q8IWB6
C	804	TYR	PRO	ENGINEERED MUTATION	UNP Q8IWB6
F	791	ASP	PRO	ENGINEERED MUTATION	UNP Q8IWB6
F	802	PRO	ILE	ENGINEERED MUTATION	UNP Q8IWB6
F	803	GLY	PRO	ENGINEERED MUTATION	UNP Q8IWB6
F	804	TYR	PRO	ENGINEERED MUTATION	UNP Q8IWB6
I	791	ASP	PRO	ENGINEERED MUTATION	UNP Q8IWB6
I	802	PRO	ILE	ENGINEERED MUTATION	UNP Q8IWB6
I	803	GLY	PRO	ENGINEERED MUTATION	UNP Q8IWB6
I	804	TYR	PRO	ENGINEERED MUTATION	UNP Q8IWB6
L	791	ASP	PRO	ENGINEERED MUTATION	UNP Q8IWB6
L	802	PRO	ILE	ENGINEERED MUTATION	UNP Q8IWB6
L	803	GLY	PRO	ENGINEERED MUTATION	UNP Q8IWB6
L	804	TYR	PRO	ENGINEERED MUTATION	UNP Q8IWB6

- Molecule 3 is water.

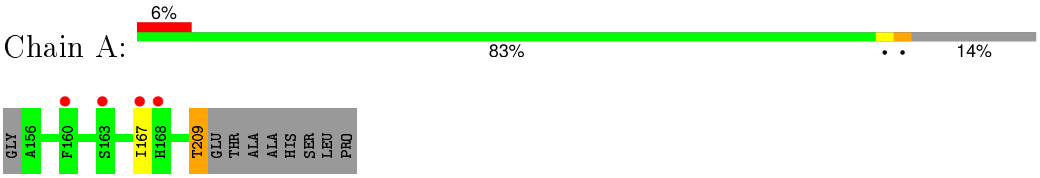
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	8	Total O 8 8	0	0
3	C	5	Total O 5 5	0	0
3	D	9	Total O 9 9	0	0
3	E	7	Total O 7 7	0	0
3	F	2	Total O 2 2	0	0
3	G	6	Total O 6 6	0	0
3	H	8	Total O 8 8	0	0
3	I	6	Total O 6 6	0	0
3	J	2	Total O 2 2	0	0
3	K	13	Total O 13 13	0	0

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 errors 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.

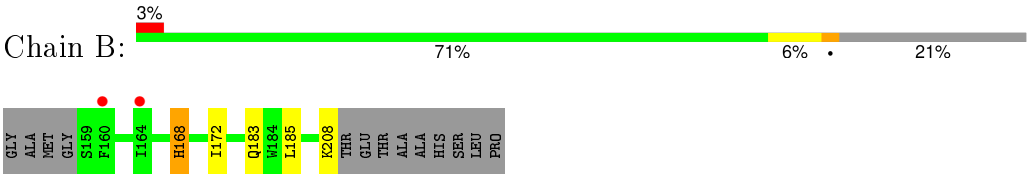
- Molecule 1: Centrosomal protein of 55 kDa

Chain A:



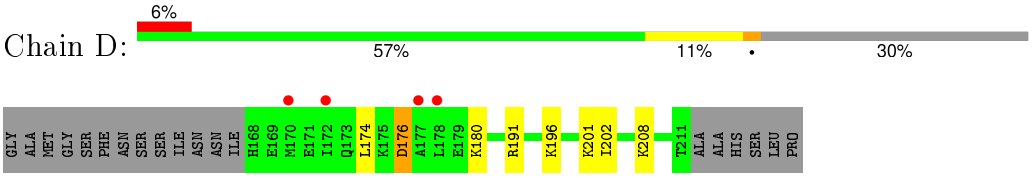
- Molecule 1: Centrosomal protein of 55 kDa

Chain B:



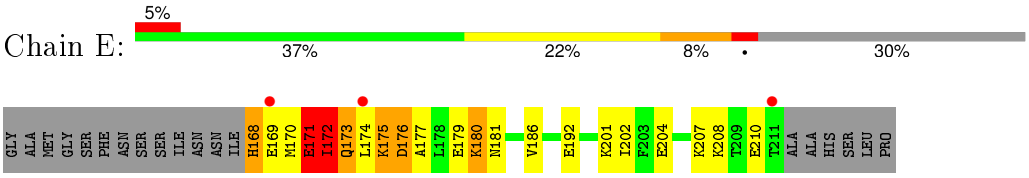
- Molecule 1: Centrosomal protein of 55 kDa

Chain D:



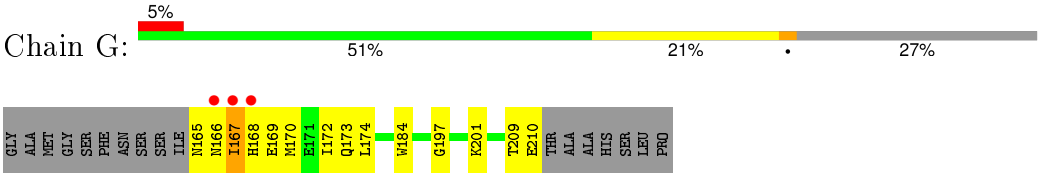
- Molecule 1: Centrosomal protein of 55 kDa

Chain E:



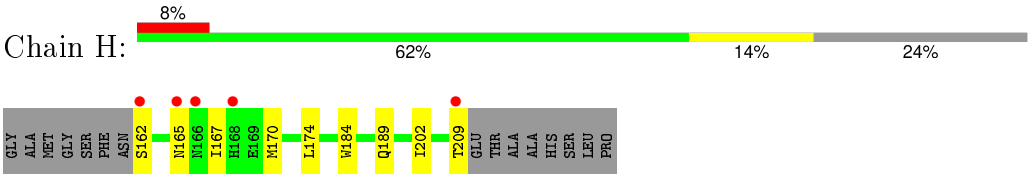
- Molecule 1: Centrosomal protein of 55 kDa

Chain G:



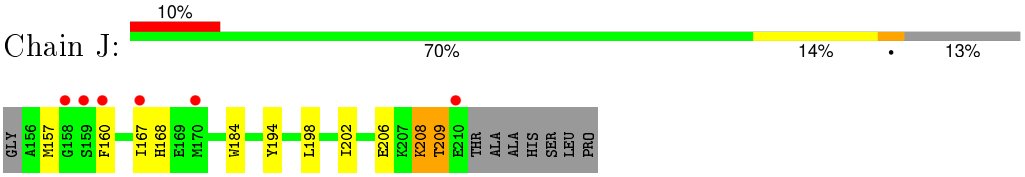
- Molecule 1: Centrosomal protein of 55 kDa

Chain H:



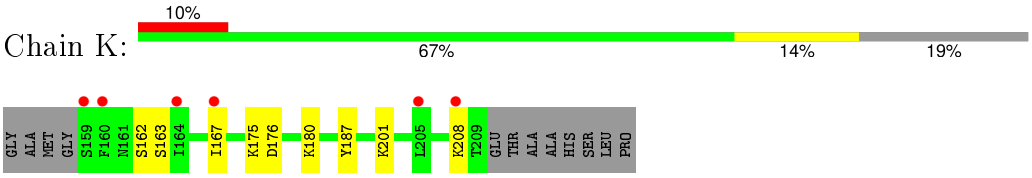
• Molecule 1: Centrosomal protein of 55 kDa

Chain J:



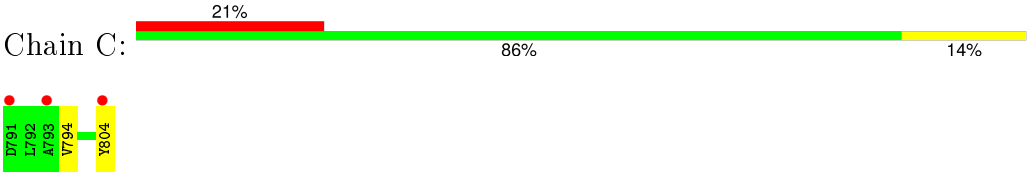
• Molecule 1: Centrosomal protein of 55 kDa

Chain K:



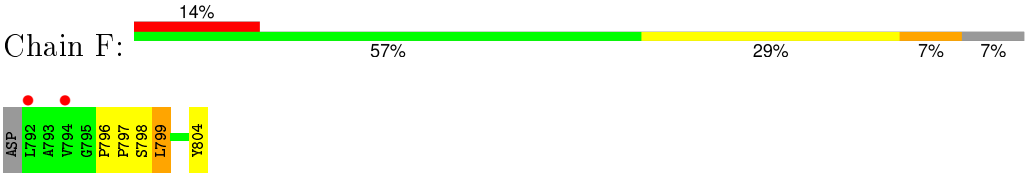
• Molecule 2: TEX-14

Chain C:



• Molecule 2: TEX-14

Chain F:

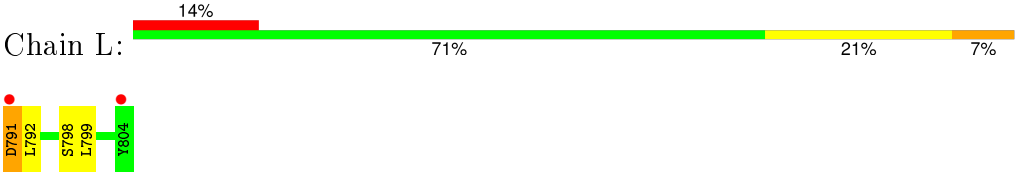


• Molecule 2: TEX-14

Chain I:

• Molecule 2: TEX-14

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.25Å 104.80Å 131.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.90 49.37 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.37-2.90) 99.6 (49.37-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	12.74 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.224 , 0.260 0.223 , 0.258	Depositor DCC
R_{free} test set	1685 reflections (10.00%)	DCC
Wilson B-factor (Å^2)	62.3	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 16868 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3787	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.25	0/453	0.38	0/606
1	B	0.24	0/429	0.33	0/574
1	D	0.24	0/382	0.45	0/511
1	E	0.59	0/382	0.73	2/511 (0.4%)
1	G	0.36	0/399	0.48	0/534
1	H	0.29	0/410	0.48	0/549
1	J	0.28	0/462	0.38	0/618
1	K	0.24	0/436	0.38	0/584
2	C	0.28	0/107	0.58	0/148
2	F	0.27	0/99	0.44	0/137
2	I	0.32	0/107	0.57	0/148
2	L	0.26	0/107	0.47	0/148
All	All	0.32	0/3773	0.47	2/5068 (0.0%)

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
1	E	0	1
1	J	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	171	GLU	N-CA-C	-7.40	91.02	111.00
1	E	172	ILE	CB-CA-C	-5.19	101.22	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	173	GLN	Peptide
1	J	208	LYS	Peptide

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	447	0	449	2	0
1	B	423	0	425	5	0
1	D	377	0	381	8	0
1	E	377	0	380	47	0
1	G	394	0	397	19	0
1	H	405	0	412	6	0
1	J	456	0	455	8	0
1	K	430	0	432	7	0
2	C	103	0	95	1	0
2	F	95	0	91	2	0
2	I	103	0	95	6	0
2	L	103	0	95	3	0
3	A	8	0	0	2	0
3	B	8	0	0	1	0
3	C	5	0	0	0	0
3	D	9	0	0	0	0
3	E	7	0	0	2	0
3	F	2	0	0	0	0
3	G	6	0	0	1	0
3	H	8	0	0	1	0
3	I	6	0	0	4	0
3	J	2	0	0	0	0
3	K	13	0	0	2	0
All	All	3787	0	3707	97	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 13.

All (97) 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:E:173:GLN:O	1:E:176:ASP:N	1.56	1.35
1:E:172:ILE:O	1:E:172:ILE:HD12	1.38	1.20
1:E:172:ILE:HG13	1:E:173:GLN:OE1	1.34	1.20
1:E:168:HIS:HE1	3:E:307:HOH:O	1.32	1.13
1:E:172:ILE:HG13	1:E:173:GLN:CD	1.73	1.08
1:E:172:ILE:C	1:E:172:ILE:HD12	1.66	1.08
1:D:174:LEU:HD11	1:E:173:GLN:HB2	1.30	1.06
1:E:172:ILE:CG1	1:E:173:GLN:OE1	2.06	1.02
1:E:173:GLN:HA	1:E:176:ASP:HB3	1.03	0.99
1:E:173:GLN:CA	1:E:176:ASP:HB3	1.92	0.99
1:E:173:GLN:HA	1:E:176:ASP:CB	1.94	0.97
1:E:172:ILE:HG13	1:E:173:GLN:N	1.80	0.96
1:E:168:HIS:HD2	1:E:168:HIS:O	1.49	0.94
1:E:172:ILE:CD1	1:E:172:ILE:C	2.30	0.93
1:E:172:ILE:HG23	1:E:173:GLN:OE1	1.69	0.92
1:G:167:ILE:CD1	1:G:167:ILE:H	1.83	0.91
1:G:167:ILE:N	1:G:167:ILE:CD1	2.34	0.90
1:E:173:GLN:O	1:E:175:LYS:N	2.07	0.88
1:G:167:ILE:HD13	1:G:167:ILE:H	1.37	0.87
1:E:170:MET:O	1:E:172:ILE:HG22	1.74	0.86
1:A:209:THR:HG22	3:A:307:HOH:O	1.74	0.86
1:E:172:ILE:CG2	1:E:173:GLN:OE1	2.23	0.85
1:G:173:GLN:NE2	2:L:791:ASP:OD1	2.10	0.84
1:E:168:HIS:CD2	1:E:168:HIS:O	2.30	0.83
1:E:172:ILE:CG1	1:E:173:GLN:CD	2.43	0.83
1:E:172:ILE:CG1	1:E:173:GLN:N	2.43	0.81
1:G:167:ILE:HD12	1:G:167:ILE:N	1.94	0.79
1:E:168:HIS:O	1:E:169:GLU:HB2	1.83	0.78
1:K:208:LYS:HB2	3:K:311:HOH:O	1.85	0.77
1:E:173:GLN:O	1:E:174:LEU:C	2.25	0.74
1:D:176:ASP:OD2	1:D:180:LYS:NZ	2.22	0.73
1:E:171:GLU:O	1:E:171:GLU:CG	2.33	0.72
1:E:171:GLU:O	1:E:171:GLU:HG3	1.88	0.72
1:D:174:LEU:CD1	1:E:173:GLN:HB2	2.17	0.72
2:I:804:TYR:CE2	3:I:906:HOH:O	2.42	0.71
1:G:168:HIS:HB3	3:G:306:HOH:O	1.91	0.70
1:E:176:ASP:OD1	1:E:176:ASP:C	2.30	0.70
1:A:209:THR:CG2	3:A:307:HOH:O	2.37	0.70
1:E:173:GLN:O	1:E:175:LYS:C	2.31	0.70
1:E:170:MET:C	1:E:172:ILE:N	2.41	0.67
1:E:170:MET:O	1:E:172:ILE:N	2.29	0.66
1:G:165:ASN:O	1:G:166:ASN:ND2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:GLN:OE1	1:E:173:GLN:N	2.30	0.64
1:E:168:HIS:CD2	1:E:168:HIS:C	2.68	0.64
2:L:791:ASP:OD1	2:L:792:LEU:N	2.31	0.63
1:G:169:GLU:HB3	1:G:172:ILE:HD13	1.83	0.60
2:I:802:PRO:C	3:I:905:HOH:O	2.40	0.60
1:E:176:ASP:OD1	1:E:180:LYS:HE2	2.02	0.59
1:G:166:ASN:OD1	1:G:170:MET:HB3	2.02	0.59
1:D:202:ILE:HD13	1:E:201:LYS:HD2	1.85	0.59
1:D:191:ARG:NH1	1:E:192:GLU:OE1	2.34	0.58
1:H:162:SER:O	1:H:165:ASN:ND2	2.38	0.57
2:L:798:SER:OG	2:L:799:LEU:N	2.39	0.56
1:G:201:LYS:HD3	1:H:202:ILE:HD13	1.88	0.56
2:I:804:TYR:N	3:I:905:HOH:O	2.38	0.56
1:B:185:LEU:HD11	2:C:794:VAL:HB	1.89	0.55
1:E:177:ALA:O	1:E:181:ASN:N	2.28	0.54
1:J:167:ILE:HD13	1:K:167:ILE:HG21	1.90	0.54
1:E:172:ILE:CB	1:E:173:GLN:OE1	2.57	0.53
1:G:165:ASN:OD1	1:G:165:ASN:C	2.47	0.53
1:G:166:ASN:O	1:G:167:ILE:C	2.43	0.52
1:E:168:HIS:CE1	3:E:307:HOH:O	2.23	0.52
2:F:798:SER:OG	2:F:799:LEU:N	2.43	0.52
1:K:176:ASP:OD1	1:K:180:LYS:NZ	2.43	0.52
1:E:171:GLU:O	1:E:171:GLU:OE2	2.29	0.51
1:D:201:LYS:HD3	1:E:202:ILE:HD13	1.94	0.49
1:B:183:GLN:HG2	1:D:196:LYS:HE2	1.94	0.49
1:E:176:ASP:O	1:E:176:ASP:OD1	2.30	0.49
1:G:165:ASN:OD1	1:G:165:ASN:O	2.30	0.48
1:G:184:TRP:HB3	1:H:184:TRP:CE3	2.48	0.48
1:G:174:LEU:HD22	1:H:170:MET:HG3	1.95	0.48
1:G:209:THR:HA	1:G:210:GLU:HA	1.65	0.47
1:G:170:MET:HB2	1:H:174:LEU:HD22	1.95	0.47
1:B:208:LYS:C	3:B:307:HOH:O	2.52	0.47
1:E:176:ASP:O	1:E:180:LYS:HB2	2.14	0.47
1:J:208:LYS:O	1:J:209:THR:OG1	2.30	0.47
1:B:183:GLN:HE21	1:D:196:LYS:HE3	1.80	0.47
1:E:173:GLN:O	1:E:175:LYS:CA	2.63	0.46
1:H:162:SER:N	3:H:307:HOH:O	2.49	0.46
1:E:204:GLU:O	1:E:207:LYS:HG2	2.14	0.46
1:E:172:ILE:HG13	1:E:173:GLN:CG	2.44	0.46
1:B:168:HIS:O	1:B:172:ILE:HG12	2.16	0.45
1:G:197:GLY:HA3	1:K:187:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:796:PRO:HG3	1:J:184:TRP:HA	2.01	0.43
1:J:194:TYR:CE2	1:J:198:LEU:HD11	2.54	0.43
2:I:801:TYR:HA	2:I:802:PRO:HA	1.84	0.43
1:E:172:ILE:HG12	1:E:173:GLN:CD	2.33	0.42
1:J:157:MET:HA	1:J:160:PHE:HD2	1.83	0.42
1:J:202:ILE:HD13	1:K:201:LYS:HD3	2.01	0.42
1:K:163:SER:O	1:K:167:ILE:HG12	2.19	0.42
1:G:172:ILE:H	1:G:172:ILE:HD12	1.84	0.42
1:E:172:ILE:HG13	1:E:173:GLN:CA	2.49	0.42
1:K:162:SER:N	3:K:310:HOH:O	2.48	0.41
2:I:803:GLY:N	3:I:905:HOH:O	2.53	0.41
1:J:198:LEU:O	1:J:202:ILE:HG13	2.20	0.41
2:F:796:PRO:HA	2:F:797:PRO:HD3	1.85	0.41
1:J:206:GLU:C	1:J:208:LYS:H	2.24	0.41

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	52/63 (82%)	52 (100%)	0	0	100	100
1	B	48/63 (76%)	48 (100%)	0	0	100	100
1	D	42/63 (67%)	40 (95%)	2 (5%)	0	100	100
1	E	42/63 (67%)	40 (95%)	2 (5%)	0	100	100
1	G	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
1	H	46/63 (73%)	43 (94%)	3 (6%)	0	100	100
1	J	53/63 (84%)	52 (98%)	1 (2%)	0	100	100
1	K	49/63 (78%)	49 (100%)	0	0	100	100
2	C	12/14 (86%)	12 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	11/14 (79%)	9 (82%)	2 (18%)	0	100	100
2	I	12/14 (86%)	12 (100%)	0	0	100	100
2	L	12/14 (86%)	12 (100%)	0	0	100	100
All	All	423/560 (76%)	410 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	49/55 (89%)	47 (96%)	2 (4%)	37	73
1	B	47/55 (86%)	46 (98%)	1 (2%)	61	88
1	D	41/55 (74%)	39 (95%)	2 (5%)	31	67
1	E	41/55 (74%)	31 (76%)	10 (24%)	1	2
1	G	43/55 (78%)	42 (98%)	1 (2%)	58	87
1	H	45/55 (82%)	42 (93%)	3 (7%)	20	50
1	J	50/55 (91%)	48 (96%)	2 (4%)	38	74
1	K	48/55 (87%)	47 (98%)	1 (2%)	61	88
2	C	11/11 (100%)	10 (91%)	1 (9%)	12	34
2	F	10/11 (91%)	8 (80%)	2 (20%)	1	5
2	I	11/11 (100%)	11 (100%)	0	100	100
2	L	11/11 (100%)	10 (91%)	1 (9%)	12	34
All	All	407/484 (84%)	381 (94%)	26 (6%)	22	53

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	ILE
1	A	209	THR

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Mol	Chain	Res	Type
1	B	168	HIS
2	C	804	TYR
1	D	176	ASP
1	D	208	LYS
1	E	168	HIS
1	E	171	GLU
1	E	172	ILE
1	E	175	LYS
1	E	176	ASP
1	E	179	GLU
1	E	180	LYS
1	E	186	VAL
1	E	208	LYS
1	E	210	GLU
2	F	799	LEU
2	F	804	TYR
1	G	167	ILE
1	H	167	ILE
1	H	189	GLN
1	H	209	THR
1	J	168	HIS
1	J	209	THR
1	K	175	LYS
2	L	791	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	168	HIS
1	H	165	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	54/63 (85%)	0.85	4 (7%) 17 11	19, 43, 74, 77	0
1	B	50/63 (79%)	0.61	2 (4%) 42 35	20, 46, 69, 75	0
1	D	44/63 (69%)	0.66	4 (9%) 11 7	21, 42, 78, 87	0
1	E	44/63 (69%)	0.67	3 (6%) 20 14	22, 48, 91, 97	0
1	G	46/63 (73%)	0.63	3 (6%) 22 16	23, 41, 77, 89	0
1	H	48/63 (76%)	0.65	5 (10%) 8 5	24, 46, 90, 99	0
1	J	55/63 (87%)	0.81	6 (10%) 7 4	27, 50, 93, 111	0
1	K	51/63 (80%)	0.76	6 (11%) 6 4	24, 44, 78, 83	0
2	C	14/14 (100%)	1.00	3 (21%) 1 0	25, 43, 80, 81	0
2	F	13/14 (92%)	0.69	2 (15%) 3 1	33, 48, 72, 85	0
2	I	14/14 (100%)	0.27	0 100 100	30, 38, 52, 65	0
2	L	14/14 (100%)	0.65	2 (14%) 4 2	35, 53, 78, 82	0
All	All	447/560 (79%)	0.70	40 (8%) 12 7	19, 46, 84, 111	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	210	GLU	4.5
1	H	165	ASN	4.2
1	A	163	SER	3.9
2	L	791	ASP	3.7
1	G	168	HIS	3.6
1	D	170	MET	3.6
1	J	170	MET	3.5
1	A	160	PHE	3.5
2	C	804	TYR	3.4
1	E	169	GLU	3.3
1	G	167	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	168	HIS	3.3
1	H	162	SER	3.2
1	K	159	SER	3.1
2	C	791	ASP	3.1
1	G	166	ASN	3.0
1	D	172	ILE	2.9
1	E	174	LEU	2.9
1	J	158	GLY	2.8
1	A	167	ILE	2.8
1	E	211	THR	2.8
1	K	167	ILE	2.7
1	K	164	ILE	2.6
1	K	160	PHE	2.6
2	F	792	LEU	2.5
2	C	793	ALA	2.5
1	J	159	SER	2.5
1	J	160	PHE	2.5
1	H	209	THR	2.4
2	L	804	TYR	2.4
1	B	160	PHE	2.4
1	K	208	LYS	2.4
1	D	178	LEU	2.4
1	B	164	ILE	2.3
1	J	167	ILE	2.3
1	H	166	ASN	2.2
1	A	168	HIS	2.2
1	K	205	LEU	2.1
1	D	177	ALA	2.1
2	F	794	VAL	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.