



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:32 PM GMT

PDB ID : 1IM3
Title : Crystal Structure of the human cytomegalovirus protein US2 bound to the MHC class I molecule HLA-A2/tax
Authors : Gewurz, B.E.; Gaudet, R.; Tortorella, D.; Wang, E.W.; Ploegh, H.L.; Wiley, D.C.
Deposited on : 2001-05-09
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

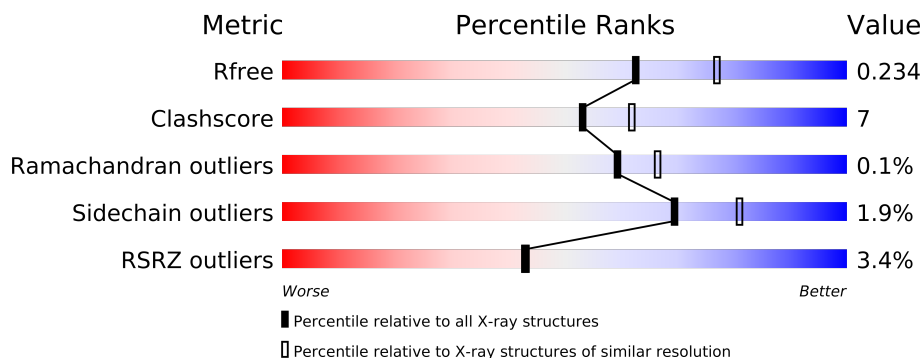
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	275	
1	E	275	
1	I	275	
1	M	275	
2	B	100	
2	F	100	
2	J	100	
2	N	100	
3	C	9	
3	G	9	
3	K	9	
3	O	9	
4	D	95	
4	H	95	

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Mol	Chain	Length	Quality of chain
4	L	95	
4	P	95	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17162 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			
1	E	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			
1	I	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			
1	M	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			

- Molecule 2 is a protein called beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	F	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	J	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	N	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	CLONING ARTIFACT	UNP P61769
F	0	MET	-	CLONING ARTIFACT	UNP P61769
J	0	MET	-	CLONING ARTIFACT	UNP P61769
N	0	MET	-	CLONING ARTIFACT	UNP P61769

- Molecule 3 is a protein called Human T-cell lymphotropic virus type 1 Tax peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			77	56	9	12			
3	G	9	Total	C	N	O	0	0	0
			77	56	9	12			
3	K	9	Total	C	N	O	0	0	0
			77	56	9	12			
3	O	9	Total	C	N	O	0	0	0
			77	56	9	12			

- Molecule 4 is a protein called cytomegalovirus protein US2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	95	Total	C	N	O	S	0	0	0
			768	497	129	138	4			
4	H	95	Total	C	N	O	S	0	0	0
			768	497	129	138	4			
4	L	95	Total	C	N	O	S	0	0	0
			768	497	129	138	4			
4	P	95	Total	C	N	O	S	0	0	0
			768	497	129	138	4			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	247	Total	O	0	0
			247	247		
5	B	63	Total	O	0	0
			63	63		
5	C	11	Total	O	0	0
			11	11		
5	D	79	Total	O	0	0
			79	79		
5	E	250	Total	O	0	0
			250	250		
5	F	67	Total	O	0	0
			67	67		
5	G	12	Total	O	0	0
			12	12		
5	H	58	Total	O	0	0
			58	58		
5	I	214	Total	O	0	0
			214	214		
5	J	60	Total	O	0	0
			60	60		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	9	Total 9	O 9	0	0
5	L	36	Total 36	O 36	0	0
5	M	220	Total 220	O 220	0	0
5	N	53	Total 53	O 53	0	0
5	O	11	Total 11	O 11	0	0
5	P	56	Total 56	O 56	0	0

3 Residue-property plots

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: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN

Chain A: 



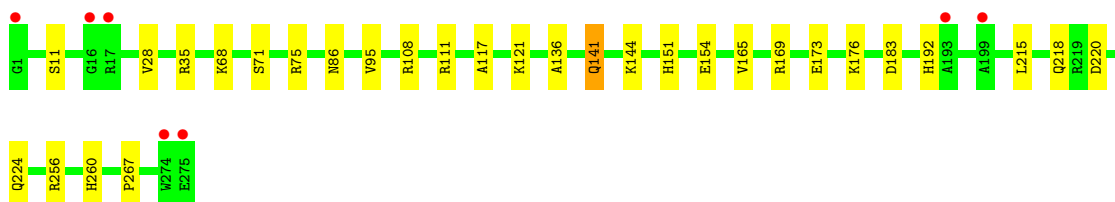
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN

Chain E: 



- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN

Chain I: 



- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN

Chain M: 



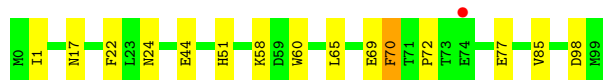
- Molecule 2: beta-2-microglobulin

Chain B: 



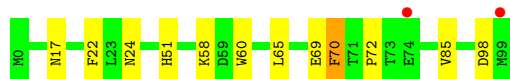
- Molecule 2: beta-2-microglobulin

Chain F: 



- Molecule 2: beta-2-microglobulin

Chain J: 



- Molecule 2: beta-2-microglobulin

Chain N: 



- Molecule 3: Human T-cell lymphotropic virus type 1 Tax peptide

Chain C: 



- Molecule 3: Human T-cell lymphotropic virus type 1 Tax peptide

Chain G: 

There are no outlier residues recorded for this chain.

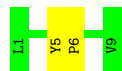
- Molecule 3: Human T-cell lymphotropic virus type 1 Tax peptide

Chain K: 

There are no outlier residues recorded for this chain.

- Molecule 3: Human T-cell lymphotropic virus type 1 Tax peptide

Chain O: 



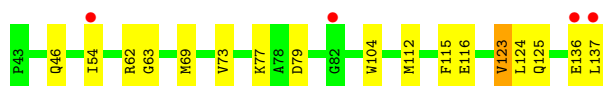
- Molecule 4: cytomegalovirus protein US2

Chain D: 



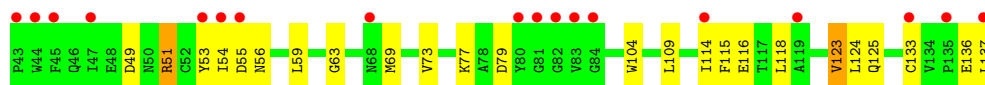
- Molecule 4: cytomegalovirus protein US2

Chain H: 



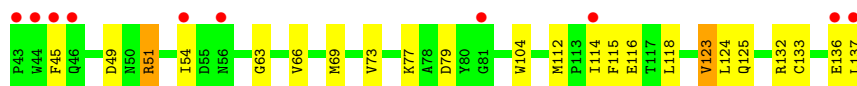
- Molecule 4: cytomagalovirus protein US2

Chain L:



- Molecule 4: cytomagalovirus protein US2

Chain P:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.48Å 96.70Å 99.54Å 109.02° 109.46° 107.93°	Depositor
Resolution (Å)	38.85 – 2.20 45.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.2 (38.85-2.20) 94.3 (45.66-2.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.20Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.206 , 0.240 0.202 , 0.234	Depositor DCC
R_{free} test set	2713 reflections (2.06%)	DCC
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.9	EDS
Estimated twinning fraction	0.013 for k,h,-h-k-l 0.010 for -k,-h,-l 0.011 for -h,-k,h+k+l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 139483 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17162	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.53	0/2312	0.70	0/3137
1	E	0.57	0/2312	0.70	1/3137 (0.0%)
1	I	0.54	0/2312	0.71	1/3137 (0.0%)
1	M	0.54	0/2312	0.70	1/3137 (0.0%)
2	B	0.48	0/860	0.67	0/1162
2	F	0.50	0/860	0.66	0/1162
2	J	0.46	0/860	0.66	0/1162
2	N	0.47	0/860	0.66	0/1162
3	C	0.59	0/80	0.86	0/108
3	G	0.61	0/80	0.88	0/108
3	K	0.69	0/80	0.84	0/108
3	O	0.71	0/80	0.84	0/108
4	D	0.54	0/788	0.82	1/1070 (0.1%)
4	H	0.50	0/788	0.72	0/1070
4	L	0.51	0/787	0.70	0/1067
4	P	0.52	0/788	0.74	0/1070
All	All	0.53	0/16159	0.71	4/21905 (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	M	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	28	VAL	N-CA-C	-5.48	96.20	111.00
1	I	28	VAL	N-CA-C	-5.33	96.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	137	LEU	CA-CB-CG	5.13	127.10	115.30
1	E	28	VAL	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	209	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2247	0	2096	29	0
1	E	2247	0	2096	27	0
1	I	2247	0	2096	25	0
1	M	2247	0	2096	32	0
2	B	837	0	803	8	0
2	F	837	0	803	13	0
2	J	837	0	803	10	0
2	N	837	0	803	7	0
3	C	77	0	79	1	0
3	G	77	0	79	0	0
3	K	77	0	79	0	0
3	O	77	0	79	2	0
4	D	768	0	746	20	0
4	H	768	0	746	14	0
4	L	768	0	745	18	0
4	P	768	0	746	22	0
5	A	247	0	0	7	0
5	B	63	0	0	1	0
5	C	11	0	0	1	0
5	D	79	0	0	4	0
5	E	250	0	0	8	0
5	F	67	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	12	0	0	0	0
5	H	58	0	0	3	0
5	I	214	0	0	4	0
5	J	60	0	0	2	0
5	K	9	0	0	0	0
5	L	36	0	0	0	0
5	M	220	0	0	5	0
5	N	53	0	0	1	0
5	O	11	0	0	1	0
5	P	56	0	0	3	0
All	All	17162	0	14895	213	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (213) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:P:69:MET:HG2	4:P:124:LEU:HB3	1.46	0.98
4:L:69:MET:HG2	4:L:124:LEU:HB3	1.45	0.98
4:D:69:MET:HG2	4:D:124:LEU:HB3	1.48	0.95
4:H:69:MET:HG2	4:H:124:LEU:HB3	1.48	0.93
4:P:73:VAL:HB	4:P:123:VAL:HG13	1.50	0.92
4:H:73:VAL:HB	4:H:123:VAL:HG13	1.52	0.92
4:L:73:VAL:HB	4:L:123:VAL:HG13	1.54	0.88
4:D:73:VAL:HB	4:D:123:VAL:HG13	1.55	0.88
1:E:192:HIS:HD2	5:E:508:HOH:O	1.61	0.82
3:C:6:PRO:HD2	5:C:1121:HOH:O	1.83	0.78
1:A:17:ARG:HB3	1:A:17:ARG:NH1	1.99	0.77
1:A:141:GLN:HE21	1:A:141:GLN:HA	1.53	0.73
4:D:49:ASP:HB2	1:M:90:ALA:HB1	1.70	0.72
2:N:3:ARG:HD3	5:N:149:HOH:O	1.90	0.71
1:E:151:HIS:HD2	1:E:154:GLU:OE2	1.75	0.69
1:M:151:HIS:HD2	1:M:154:GLU:OE2	1.76	0.68
1:I:151:HIS:HD2	1:I:154:GLU:OE2	1.76	0.68
4:P:69:MET:HG3	5:P:192:HOH:O	1.94	0.67
1:I:141:GLN:HE22	1:I:144:LYS:HD3	1.61	0.66
4:H:54:ILE:HD11	4:H:115:PHE:CD2	2.30	0.66
1:A:141:GLN:HE22	1:A:144:LYS:HD3	1.60	0.66
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.31	0.65
1:E:173:GLU:OE2	1:E:176:LYS:HE3	1.95	0.65
1:M:117:ALA:HB2	2:N:60:TRP:CE2	2.32	0.65
1:A:17:ARG:HH11	1:A:17:ARG:HB3	1.59	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:117:ALA:HB2	2:J:60:TRP:CE2	2.33	0.64
4:L:51:ARG:HG2	4:L:51:ARG:HH11	1.63	0.64
1:A:151:HIS:HD2	1:A:154:GLU:OE2	1.81	0.63
4:L:54:ILE:HD11	4:L:115:PHE:CD2	2.34	0.63
5:D:149:HOH:O	1:M:88:SER:HB3	1.99	0.62
1:E:35:ARG:CZ	5:E:454:HOH:O	2.48	0.62
2:J:58:LYS:HE2	5:J:133:HOH:O	1.97	0.62
1:I:111:ARG:HG3	5:I:304:HOH:O	1.99	0.62
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.35	0.61
1:I:141:GLN:HE21	1:I:141:GLN:HA	1.64	0.61
4:P:136:GLU:O	4:P:137:LEU:HB2	2.01	0.61
4:H:63:GLY:HA3	4:H:104:TRP:CZ2	2.38	0.58
1:A:141:GLN:NE2	1:A:141:GLN:HA	2.18	0.58
1:E:141:GLN:HE21	1:E:141:GLN:HA	1.67	0.58
1:E:141:GLN:HE22	1:E:144:LYS:HD3	1.69	0.58
2:J:85:VAL:HG22	5:J:107:HOH:O	2.02	0.58
1:M:173:GLU:OE2	1:M:176:LYS:HE3	2.05	0.57
2:F:44:GLU:HG2	5:F:151:HOH:O	2.04	0.57
1:I:173:GLU:OE2	1:I:176:LYS:HE3	2.03	0.56
1:E:192:HIS:CD2	5:E:508:HOH:O	2.45	0.56
4:D:58:LYS:HD3	4:D:108:ASN:OD1	2.05	0.56
1:A:253:GLN:HG2	1:I:136:ALA:O	2.05	0.56
1:M:35:ARG:NH2	5:M:424:HOH:O	2.38	0.56
4:P:69:MET:HA	4:P:125:GLN:HG2	1.88	0.56
4:P:51:ARG:HG2	4:P:51:ARG:HH11	1.69	0.56
1:M:141:GLN:HE21	1:M:141:GLN:HA	1.69	0.56
4:L:63:GLY:HA3	4:L:104:TRP:CZ2	2.41	0.56
1:A:35:ARG:CZ	5:A:366:HOH:O	2.53	0.55
5:E:484:HOH:O	2:F:58:LYS:HE3	2.06	0.55
4:L:136:GLU:C	4:L:137:LEU:HD23	2.27	0.55
4:H:63:GLY:HA3	4:H:104:TRP:CE2	2.43	0.54
1:E:192:HIS:CE1	2:F:98:ASP:HB3	2.43	0.54
1:M:141:GLN:HE22	1:M:144:LYS:HD3	1.73	0.54
4:P:63:GLY:HA3	4:P:104:TRP:CZ2	2.43	0.53
1:A:173:GLU:OE2	1:A:176:LYS:HE3	2.08	0.53
4:L:59:LEU:HD23	4:L:109:LEU:HD23	1.90	0.53
1:I:141:GLN:NE2	1:I:141:GLN:HA	2.23	0.53
4:D:63:GLY:HA3	4:D:104:TRP:CZ2	2.44	0.53
1:A:218:GLN:HG3	1:A:260:HIS:CD2	2.43	0.53
4:H:62:ARG:HD3	5:H:177:HOH:O	2.08	0.53
1:A:141:GLN:HE21	1:A:141:GLN:CA	2.16	0.52
1:E:35:ARG:NH2	5:E:454:HOH:O	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:77:GLU:HG2	5:F:154:HOH:O	2.09	0.52
1:A:35:ARG:NH2	5:A:366:HOH:O	2.43	0.52
1:I:141:GLN:HE21	1:I:141:GLN:CA	2.22	0.51
4:L:63:GLY:HA3	4:L:104:TRP:CE2	2.45	0.51
1:I:75:ARG:HG2	1:I:75:ARG:HH11	1.77	0.50
4:H:69:MET:HA	4:H:125:GLN:HG2	1.92	0.50
1:M:35:ARG:CZ	5:M:424:HOH:O	2.59	0.50
1:M:75:ARG:HG2	1:M:75:ARG:HH11	1.74	0.50
4:P:54:ILE:HD11	4:P:115:PHE:CD2	2.47	0.50
4:P:69:MET:HA	4:P:125:GLN:CG	2.41	0.50
1:E:11:SER:HB3	1:E:95:VAL:HG12	1.94	0.50
1:E:75:ARG:HG2	1:E:75:ARG:HH11	1.76	0.50
1:E:141:GLN:HE21	1:E:141:GLN:CA	2.24	0.50
1:E:111:ARG:HG3	5:E:287:HOH:O	2.10	0.50
1:I:218:GLN:HG3	1:I:260:HIS:CD2	2.46	0.50
4:H:69:MET:HA	4:H:125:GLN:CG	2.41	0.50
4:P:112:MET:O	4:P:115:PHE:HB2	2.11	0.50
4:D:63:GLY:HA3	4:D:104:TRP:CE2	2.47	0.50
1:E:253:GLN:HG2	1:M:136:ALA:O	2.12	0.50
1:M:141:GLN:NE2	1:M:141:GLN:HA	2.27	0.49
1:E:141:GLN:NE2	1:E:141:GLN:HA	2.27	0.49
1:E:11:SER:HB3	1:E:95:VAL:CG1	2.42	0.49
1:A:75:ARG:HH11	1:A:75:ARG:HG2	1.77	0.49
1:A:226:GLN:HA	5:A:428:HOH:O	2.12	0.49
1:M:192:HIS:CE1	2:N:98:ASP:HB3	2.46	0.49
4:P:49:ASP:OD1	4:P:51:ARG:NE	2.45	0.49
4:P:123:VAL:HG22	5:P:145:HOH:O	2.11	0.49
1:I:11:SER:HB3	1:I:95:VAL:CG1	2.43	0.49
4:P:45:PHE:HA	4:P:66:VAL:O	2.13	0.49
1:A:255:GLN:HG3	5:A:521:HOH:O	2.13	0.49
4:P:63:GLY:HA3	4:P:104:TRP:CE2	2.47	0.49
1:I:192:HIS:CE1	2:J:98:ASP:HB3	2.48	0.48
4:L:49:ASP:OD1	4:L:51:ARG:HD3	2.14	0.48
1:M:253:GLN:OE1	1:M:256:ARG:NH1	2.42	0.48
1:A:11:SER:HB3	1:A:95:VAL:CG1	2.44	0.48
1:M:220:ASP:OD2	1:M:256:ARG:NH2	2.37	0.48
1:A:72:GLN:HB2	5:A:468:HOH:O	2.14	0.47
4:D:44:TRP:HA	5:D:156:HOH:O	2.14	0.47
4:L:69:MET:HA	4:L:125:GLN:CG	2.44	0.47
1:I:11:SER:HB3	1:I:95:VAL:HG12	1.96	0.47
1:A:220:ASP:OD2	1:A:256:ARG:NH2	2.34	0.47
4:D:103:LYS:HE2	5:D:184:HOH:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:218:GLN:HG3	1:E:260:HIS:CD2	2.49	0.47
4:L:69:MET:HA	4:L:125:GLN:HG2	1.97	0.47
1:M:141:GLN:HE21	1:M:141:GLN:CA	2.25	0.47
1:A:192:HIS:CE1	2:B:98:ASP:HB3	2.49	0.47
4:D:88:TYR:HA	5:D:159:HOH:O	2.14	0.47
4:D:69:MET:HA	4:D:125:GLN:CG	2.45	0.46
1:E:192:HIS:HB3	5:E:394:HOH:O	2.16	0.46
2:N:51:HIS:HA	2:N:65:LEU:O	2.16	0.46
1:A:75:ARG:NH2	5:A:377:HOH:O	2.48	0.46
2:B:51:HIS:HA	2:B:65:LEU:O	2.15	0.46
1:M:218:GLN:HG3	1:M:260:HIS:CD2	2.50	0.46
1:E:220:ASP:OD2	1:E:256:ARG:NH2	2.39	0.46
1:I:86:ASN:HD22	1:I:86:ASN:N	2.14	0.46
2:J:51:HIS:HA	2:J:65:LEU:O	2.16	0.46
4:D:79:ASP:O	4:D:116:GLU:HB2	2.15	0.46
2:F:22:PHE:CE2	2:F:69:GLU:HG2	2.50	0.46
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.98	0.45
4:D:114:ILE:HG13	4:D:114:ILE:H	1.60	0.45
2:F:51:HIS:HA	2:F:65:LEU:O	2.16	0.45
4:H:46:GLN:NE2	5:H:173:HOH:O	2.50	0.45
1:M:224:GLN:HE21	1:M:224:GLN:HB3	1.51	0.45
4:D:69:MET:HA	4:D:125:GLN:HG2	1.98	0.45
2:B:17:ASN:HA	2:B:72:PRO:O	2.16	0.45
4:H:136:GLU:O	4:H:137:LEU:HD23	2.16	0.45
1:M:11:SER:HB3	1:M:95:VAL:CG1	2.46	0.45
1:A:141:GLN:NE2	1:A:144:LYS:HD3	2.29	0.45
4:P:49:ASP:CG	4:P:51:ARG:HE	2.20	0.45
1:E:151:HIS:CD2	1:E:154:GLU:OE2	2.65	0.45
1:A:11:SER:HB3	1:A:95:VAL:HG12	1.99	0.45
4:L:79:ASP:O	4:L:116:GLU:HB2	2.17	0.45
4:L:55:ASP:O	4:L:56:ASN:HB3	2.16	0.45
2:F:17:ASN:HA	2:F:72:PRO:O	2.17	0.44
4:P:79:ASP:O	4:P:116:GLU:HB2	2.16	0.44
4:D:58:LYS:HB3	4:D:108:ASN:HA	1.98	0.44
1:M:75:ARG:HG2	1:M:75:ARG:NH1	2.32	0.44
1:M:74:HIS:CD2	5:M:312:HOH:O	2.70	0.44
3:O:6:PRO:HD2	5:O:848:HOH:O	2.17	0.44
2:B:70:PHE:CZ	2:B:72:PRO:HG3	2.52	0.44
1:M:165:VAL:O	1:M:169:ARG:HG3	2.17	0.44
1:E:224:GLN:HB3	1:E:224:GLN:HE21	1.51	0.43
4:D:59:LEU:HB3	4:D:109:LEU:HB3	2.01	0.43
2:F:1:ILE:HD11	1:M:250:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:L:51:ARG:NH1	4:L:51:ARG:HG2	2.30	0.43
4:D:58:LYS:CD	4:D:108:ASN:OD1	2.66	0.43
3:O:5:TYR:HA	3:O:6:PRO:HD3	1.84	0.43
4:P:114:ILE:H	4:P:114:ILE:HG13	1.62	0.43
4:H:79:ASP:O	4:H:116:GLU:HB2	2.18	0.43
1:A:46:GLU:HB3	5:A:458:HOH:O	2.19	0.43
1:E:68:LYS:O	1:E:71:SER:HB3	2.19	0.43
1:I:117:ALA:HB2	2:J:60:TRP:CD2	2.54	0.43
4:P:136:GLU:HG3	5:P:157:HOH:O	2.18	0.43
1:M:72:GLN:HB2	5:M:450:HOH:O	2.19	0.43
2:J:70:PHE:CZ	2:J:72:PRO:HG3	2.54	0.43
2:J:17:ASN:HA	2:J:72:PRO:O	2.19	0.43
4:D:59:LEU:N	4:D:109:LEU:O	2.44	0.43
4:H:69:MET:CG	4:H:124:LEU:HB3	2.33	0.42
4:H:123:VAL:HG22	5:H:142:HOH:O	2.19	0.42
1:E:192:HIS:HE1	2:F:98:ASP:HB3	1.82	0.42
1:E:75:ARG:NH1	1:E:75:ARG:HG2	2.34	0.42
1:A:75:ARG:HG2	1:A:75:ARG:NH1	2.34	0.42
2:N:24:ASN:HB3	2:N:65:LEU:HD11	2.02	0.42
2:J:24:ASN:HB3	2:J:65:LEU:HD11	2.02	0.42
4:P:132:ARG:HG2	4:P:132:ARG:NH1	2.34	0.42
1:I:68:LYS:O	1:I:71:SER:HB3	2.20	0.42
1:I:141:GLN:NE2	1:I:144:LYS:HD3	2.30	0.42
4:L:118:LEU:HB3	4:L:133:CYS:HB3	2.02	0.42
4:D:54:ILE:HD11	4:D:115:PHE:CD2	2.55	0.42
1:M:33:PHE:CD2	1:M:34:VAL:HG13	2.55	0.42
4:P:51:ARG:NH1	4:P:51:ARG:HG2	2.34	0.42
4:L:114:ILE:H	4:L:114:ILE:HG13	1.61	0.42
1:M:68:LYS:O	1:M:71:SER:HB3	2.19	0.42
1:M:264:GLU:HG3	5:M:280:HOH:O	2.19	0.42
2:F:70:PHE:CZ	2:F:72:PRO:HG3	2.55	0.41
2:B:22:PHE:CE2	2:B:69:GLU:HG2	2.55	0.41
1:A:17:ARG:CB	1:A:17:ARG:CZ	2.99	0.41
1:I:165:VAL:O	1:I:169:ARG:HG3	2.21	0.41
1:M:196:ASP:OD1	1:M:196:ASP:O	2.39	0.41
2:N:70:PHE:CZ	2:N:72:PRO:HG3	2.56	0.41
1:M:117:ALA:HB2	2:N:60:TRP:CD2	2.55	0.41
2:F:24:ASN:HB3	2:F:65:LEU:HD11	2.03	0.41
1:M:11:SER:HB3	1:M:95:VAL:HG12	2.03	0.41
1:E:165:VAL:O	1:E:169:ARG:HG3	2.21	0.41
1:I:108:ARG:HD2	5:I:414:HOH:O	2.20	0.41
1:M:111:ARG:HG2	1:M:112:GLY:N	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:267:PRO:HD2	5:E:336:HOH:O	2.21	0.41
1:I:220:ASP:OD2	1:I:256:ARG:NH2	2.38	0.41
4:P:118:LEU:HB3	4:P:133:CYS:HB3	2.03	0.41
1:I:267:PRO:HD2	5:I:448:HOH:O	2.21	0.41
2:J:22:PHE:CE2	2:J:69:GLU:HG2	2.55	0.41
1:M:15:PRO:HG2	1:M:91:GLY:O	2.20	0.41
1:I:151:HIS:CD2	1:I:154:GLU:OE2	2.65	0.41
4:H:112:MET:O	4:H:115:PHE:HB2	2.21	0.41
1:I:35:ARG:CZ	5:I:412:HOH:O	2.69	0.41
2:F:85:VAL:HG22	5:F:114:HOH:O	2.20	0.40
4:D:69:MET:CG	4:D:124:LEU:HB3	2.35	0.40
4:L:136:GLU:C	4:L:137:LEU:N	2.75	0.40
1:I:75:ARG:NH1	1:I:75:ARG:HG2	2.35	0.40
4:P:45:PHE:C	4:P:45:PHE:CD1	2.95	0.40
1:A:215:LEU:HD22	1:A:243:LYS:HD3	2.04	0.40
4:D:118:LEU:HB3	4:D:133:CYS:HB3	2.04	0.40
4:L:53:TYR:HB2	4:L:137:LEU:N	2.37	0.40
2:B:16:GLU:HA	5:B:161:HOH:O	2.19	0.40
1:A:224:GLN:HE21	1:A:224:GLN:HB3	1.53	0.40
1:A:114:HIS:CG	1:A:156:LEU:HD13	2.57	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	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
1	E	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
1	I	273/275 (99%)	269 (98%)	4 (2%)	0	100	100
1	M	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	F	98/100 (98%)	95 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	N	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	G	7/9 (78%)	7 (100%)	0	0	100	100
3	K	7/9 (78%)	7 (100%)	0	0	100	100
3	O	7/9 (78%)	7 (100%)	0	0	100	100
4	D	93/95 (98%)	85 (91%)	7 (8%)	1 (1%)	21	16
4	H	93/95 (98%)	82 (88%)	11 (12%)	0	100	100
4	L	92/95 (97%)	84 (91%)	8 (9%)	0	100	100
4	P	93/95 (98%)	86 (92%)	7 (8%)	0	100	100
All	All	1883/1916 (98%)	1818 (96%)	64 (3%)	1 (0%)	59	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	50	ASN

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	231/231 (100%)	227 (98%)	4 (2%)	73	84
1	E	231/231 (100%)	227 (98%)	4 (2%)	73	84
1	I	231/231 (100%)	226 (98%)	5 (2%)	64	76
1	M	231/231 (100%)	226 (98%)	5 (2%)	64	76
2	B	95/95 (100%)	94 (99%)	1 (1%)	84	92
2	F	95/95 (100%)	94 (99%)	1 (1%)	84	92
2	J	95/95 (100%)	94 (99%)	1 (1%)	84	92
2	N	95/95 (100%)	94 (99%)	1 (1%)	84	92
3	C	8/8 (100%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	8/8 (100%)	8 (100%)	0	100	100
3	K	8/8 (100%)	8 (100%)	0	100	100
3	O	8/8 (100%)	8 (100%)	0	100	100
4	D	83/83 (100%)	81 (98%)	2 (2%)	61	73
4	H	83/83 (100%)	81 (98%)	2 (2%)	61	73
4	L	83/83 (100%)	80 (96%)	3 (4%)	47	56
4	P	83/83 (100%)	80 (96%)	3 (4%)	47	56
All	All	1668/1668 (100%)	1636 (98%)	32 (2%)	69	81

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LYS
1	A	141	GLN
1	A	183	ASP
1	A	224	GLN
2	B	70	PHE
4	D	77	LYS
4	D	123	VAL
1	E	121	LYS
1	E	141	GLN
1	E	183	ASP
1	E	224	GLN
2	F	70	PHE
4	H	77	LYS
4	H	123	VAL
1	I	121	LYS
1	I	141	GLN
1	I	183	ASP
1	I	215	LEU
1	I	224	GLN
2	J	70	PHE
4	L	51	ARG
4	L	77	LYS
4	L	123	VAL
1	M	88	SER
1	M	121	LYS
1	M	141	GLN
1	M	183	ASP
1	M	224	GLN

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Mol	Chain	Res	Type
2	N	70	PHE
4	P	51	ARG
4	P	77	LYS
4	P	123	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	151	HIS
2	B	2	GLN
1	E	74	HIS
1	E	141	GLN
1	E	151	HIS
1	E	224	GLN
2	F	2	GLN
1	I	86	ASN
1	I	141	GLN
1	I	151	HIS
2	J	2	GLN
4	L	46	GLN
1	M	141	GLN
1	M	151	HIS
1	M	224	GLN
2	N	2	GLN
4	P	125	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 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, 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	275/275 (100%)	-0.24	2 (0%) 84 86	19, 33, 52, 75	0
1	E	275/275 (100%)	-0.26	4 (1%) 70 71	17, 32, 53, 76	0
1	I	275/275 (100%)	-0.13	7 (2%) 54 55	22, 35, 54, 73	0
1	M	275/275 (100%)	-0.10	5 (1%) 65 66	21, 34, 54, 76	0
2	B	100/100 (100%)	0.05	3 (3%) 48 48	24, 43, 72, 82	0
2	F	100/100 (100%)	-0.09	1 (1%) 79 80	20, 42, 69, 81	0
2	J	100/100 (100%)	0.02	2 (2%) 62 62	23, 44, 72, 82	0
2	N	100/100 (100%)	0.21	3 (3%) 48 48	24, 44, 72, 82	0
3	C	9/9 (100%)	-0.50	0 100 100	24, 29, 37, 49	0
3	G	9/9 (100%)	-0.39	0 100 100	21, 28, 36, 49	0
3	K	9/9 (100%)	-0.19	0 100 100	25, 29, 37, 48	0
3	O	9/9 (100%)	-0.33	0 100 100	23, 28, 36, 47	0
4	D	95/95 (100%)	0.46	6 (6%) 19 19	26, 42, 67, 85	0
4	H	95/95 (100%)	0.28	4 (4%) 35 35	25, 46, 69, 86	0
4	L	95/95 (100%)	0.86	18 (18%) 2 2	29, 49, 71, 91	0
4	P	95/95 (100%)	0.56	10 (10%) 7 6	27, 45, 68, 86	0
All	All	1916/1916 (100%)	0.01	65 (3%) 43 43	17, 37, 67, 91	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	137	LEU	8.6
4	D	137	LEU	7.8
4	P	137	LEU	7.2
4	L	43	PRO	7.2
4	P	43	PRO	7.0

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Mol	Chain	Res	Type	RSRZ
4	L	137	LEU	6.6
4	L	44	TRP	5.0
1	A	1	GLY	4.0
1	I	16	GLY	4.0
4	L	83	VAL	3.9
1	E	275	GLU	3.8
2	N	99	MET	3.8
2	J	99	MET	3.7
4	D	43	PRO	3.7
1	A	275	GLU	3.7
2	N	75	LYS	3.6
4	P	44	TRP	3.6
4	L	84	GLY	3.6
1	I	1	GLY	3.5
4	L	80	TYR	3.5
2	N	74	GLU	3.4
4	H	136	GLU	3.3
4	P	136	GLU	3.2
1	E	1	GLY	3.2
4	L	45	PHE	3.1
4	P	45	PHE	3.0
4	D	56	ASN	3.0
4	L	47	ILE	3.0
4	H	82	GLY	3.0
1	I	199	ALA	2.9
1	M	275	GLU	2.8
1	E	192	HIS	2.8
2	B	75	LYS	2.8
4	L	114	ILE	2.8
4	P	46	GLN	2.8
4	L	82	GLY	2.7
2	F	74	GLU	2.7
4	L	135	PRO	2.7
4	L	133	CYS	2.6
1	M	192	HIS	2.6
1	E	194	VAL	2.6
4	L	119	ALA	2.6
1	M	16	GLY	2.6
4	P	54	ILE	2.6
4	P	114	ILE	2.6
4	L	81	GLY	2.6
4	D	53	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	1	GLY	2.5
2	J	74	GLU	2.4
4	L	54	ILE	2.4
1	M	194	VAL	2.4
1	I	17	ARG	2.4
4	P	81	GLY	2.3
1	I	275	GLU	2.3
4	D	136	GLU	2.3
1	I	274	TRP	2.3
4	P	56	ASN	2.3
4	L	55	ASP	2.3
4	H	54	ILE	2.2
4	L	68	ASN	2.2
2	B	74	GLU	2.1
1	I	193	ALA	2.1
4	D	133	CYS	2.1
2	B	16	GLU	2.1
4	L	53	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.