



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:16 am GMT

PDB ID : 4F7M  
Title : Crystal Structure of HLA-A\*2402 Complexed with a Newly Identified Peptide from 2009 H1N1 PA (649-658)  
Authors : Liu, J.; Zhang, S.; Tan, S.; Yi, Y.; Wu, B.; Zhu, F.; Wang, H.; Qi, J.; George, F.G.  
Deposited on : 2012-05-16  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

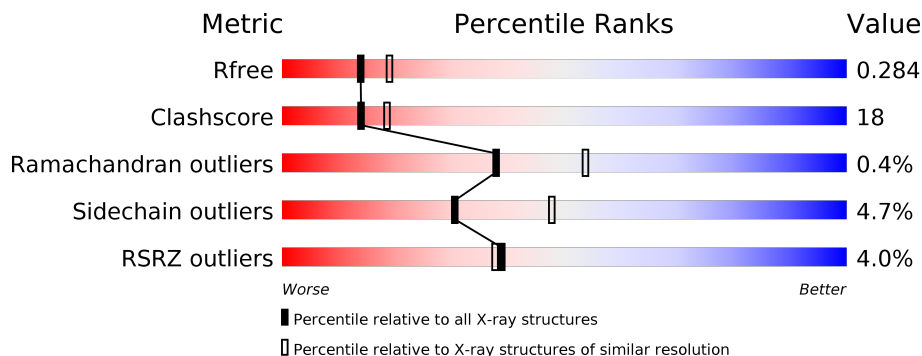
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>.</div> </div> </div>
1	D	275	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>.</div> </div> </div>
2	B	100	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>34%</div> <div>.</div> </div> </div>
2	E	100	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>.</div> </div> </div>
3	C	10	<div> <div></div> <div> <div>40%</div> <div>50%</div> <div>10%</div> </div> </div>
3	F	10	<div> <div>20%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6673 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 HLA class I histocompatibility antigen, A-24 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2222	1382	403	427	10			
1	D	274	Total	C	N	O	S	0	0	0
			2222	1382	403	427	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	UNP P05534
D	0	MET	-	INITIATING METHIONINE	UNP P05534

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	E	99	Total	C	N	O	S	0	1	0
			838	534	142	159	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769
E	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called PA polymerase subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			80	53	11	16			
3	F	10	Total	C	N	O	0	0	0
			80	53	11	16			

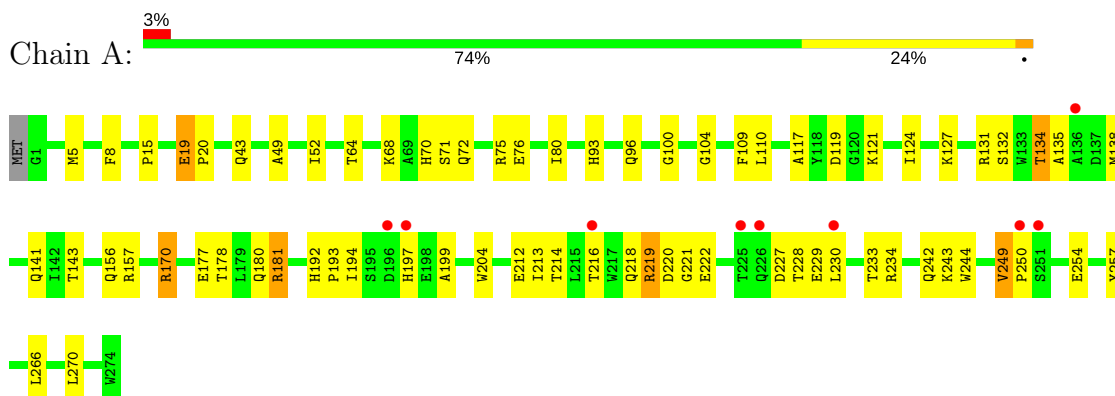
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total 133	O 133	0	0
4	B	89	Total 89	O 89	0	0
4	C	5	Total 5	O 5	0	0
4	D	110	Total 110	O 110	0	0
4	E	63	Total 63	O 63	0	0
4	F	2	Total 2	O 2	0	0

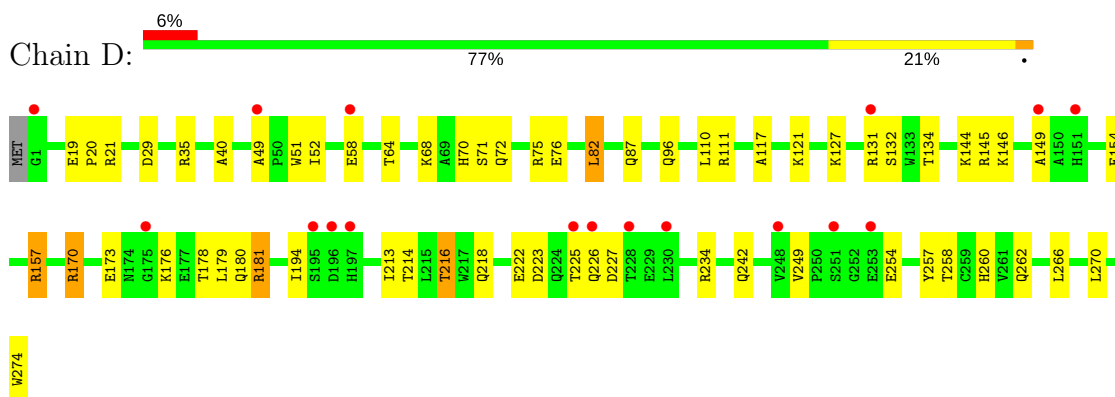
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

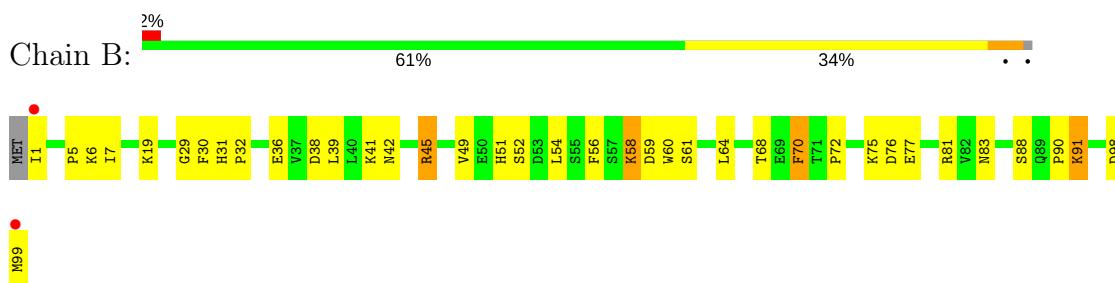
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain



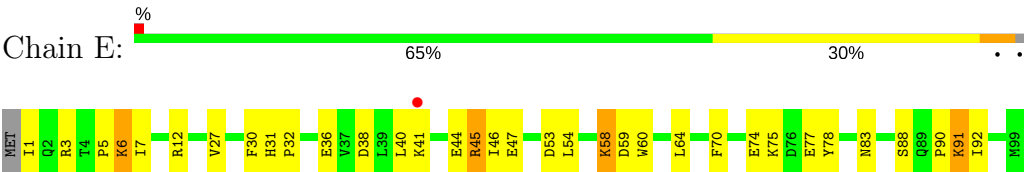
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain



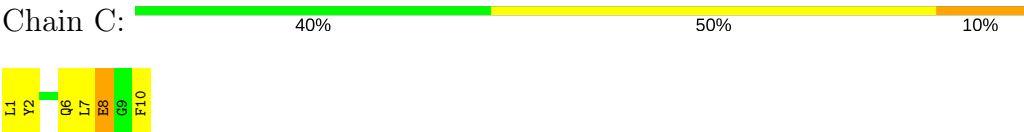
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



• Molecule 3: PA polymerase subunit



• Molecule 3: PA polymerase subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.27Å 67.09Å 87.67Å 90.00° 101.30° 90.00°	Depositor
Resolution (Å)	40.67 – 2.40 42.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.9 (40.67-2.40) 99.5 (42.98-2.40)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.239 , 0.289 0.236 , 0.284	Depositor DCC
$R_{free}$ test set	1668 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.56 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.0978e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0/2282	0.42	0/3092
1	D	0.27	0/2282	0.41	0/3092
2	B	0.37	0/852	0.46	0/1152
2	E	0.24	0/861	0.40	0/1163
3	C	0.45	0/82	0.55	0/109
3	F	0.25	0/82	0.38	0/109
All	All	0.28	0/6441	0.42	0/8717

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	2222	0	2082	69	0
1	D	2222	0	2082	67	0
2	B	829	0	794	41	0
2	E	838	0	806	37	0
3	C	80	0	76	13	0
3	F	80	0	76	6	0
4	A	133	0	0	34	1
4	B	89	0	0	18	1
4	C	5	0	0	3	0
4	D	110	0	0	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	63	0	0	14	0
4	F	2	0	0	0	0
All	All	6673	0	5916	215	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 18.

All (215) 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:D:58:GLU:HG2	4:D:376:HOH:O	1.28	1.33
1:D:58:GLU:HB3	4:D:380:HOH:O	1.23	1.32
2:B:68:THR:CB	4:B:180:HOH:O	1.90	1.16
1:A:135:ALA:HA	4:A:421:HOH:O	1.46	1.15
1:A:124:ILE:HA	4:A:421:HOH:O	1.51	1.11
1:A:219:ARG:HG2	1:A:219:ARG:HH11	1.00	1.10
2:B:41:LYS:HA	4:B:183:HOH:O	1.50	1.10
1:A:110:LEU:C	4:A:423:HOH:O	1.93	1.06
2:E:31:HIS:HB3	4:E:145:HOH:O	1.57	1.04
1:A:228:THR:C	4:A:394:HOH:O	1.95	1.02
1:D:75:ARG:NH1	4:D:350:HOH:O	1.92	1.02
1:A:244:TRP:NE1	4:A:397:HOH:O	1.91	1.02
1:D:75:ARG:NH2	4:D:350:HOH:O	1.96	0.99
2:B:68:THR:HB	4:B:180:HOH:O	1.57	0.99
1:A:134:THR:O	4:A:421:HOH:O	1.81	0.99
1:A:250:PRO:HD2	4:A:419:HOH:O	1.61	0.99
2:B:88:SER:OG	4:B:166:HOH:O	1.82	0.97
1:A:229:GLU:N	4:A:394:HOH:O	1.94	0.97
3:C:7:LEU:HG	3:C:8:GLU:H	1.30	0.96
1:D:75:ARG:CZ	4:D:350:HOH:O	2.11	0.96
2:B:77:GLU:O	4:B:183:HOH:O	1.82	0.96
1:A:219:ARG:HG2	1:A:219:ARG:NH1	1.70	0.95
2:E:3:ARG:N	4:E:145:HOH:O	1.93	0.93
2:E:12:ARG:O	4:E:160:HOH:O	1.87	0.92
1:A:204:TRP:HZ2	4:B:163:HOH:O	1.58	0.87
1:D:222:GLU:O	4:D:374:HOH:O	1.94	0.86
1:D:222:GLU:C	4:D:374:HOH:O	2.13	0.86
1:A:19:GLU:HG3	1:A:75:ARG:HD2	1.58	0.84
1:A:110:LEU:O	4:A:423:HOH:O	1.93	0.84
2:E:31:HIS:O	4:E:145:HOH:O	1.95	0.83
1:D:225:THR:HG23	4:D:399:HOH:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:ARG:O	4:D:312:HOH:O	1.96	0.83
1:D:58:GLU:CB	4:D:380:HOH:O	1.97	0.82
1:D:223:ASP:C	4:D:374:HOH:O	2.17	0.82
2:B:42:ASN:N	4:B:183:HOH:O	2.01	0.81
1:D:110:LEU:C	4:D:369:HOH:O	2.19	0.81
1:A:228:THR:CA	4:A:394:HOH:O	2.28	0.81
1:A:219:ARG:CG	1:A:219:ARG:HH11	1.89	0.80
2:E:83:ASN:HD21	2:E:90:PRO:HG3	1.46	0.80
1:A:194:ILE:HG13	4:A:353:HOH:O	1.80	0.80
1:D:227:ASP:OD1	4:D:370:HOH:O	2.00	0.80
1:A:157:ARG:NH2	4:A:416:HOH:O	2.13	0.80
1:A:227:ASP:O	4:A:394:HOH:O	2.01	0.79
2:E:31:HIS:CB	4:E:145:HOH:O	2.22	0.78
4:A:397:HOH:O	2:B:99:MET:O	2.02	0.77
1:A:181:ARG:NH1	4:A:396:HOH:O	2.17	0.77
1:A:199:ALA:HA	4:A:353:HOH:O	1.83	0.77
1:D:257:TYR:OH	4:D:383:HOH:O	1.94	0.76
2:E:77:GLU:HB3	4:E:144:HOH:O	1.83	0.76
2:B:98:ASP:C	4:B:163:HOH:O	2.24	0.76
1:A:249:VAL:HG21	1:A:254:GLU:HG3	1.69	0.75
2:B:83:ASN:HD21	2:B:90:PRO:HG3	1.51	0.75
1:D:176:LYS:NZ	4:D:381:HOH:O	2.14	0.75
1:A:250:PRO:CD	4:A:419:HOH:O	2.28	0.74
3:C:7:LEU:HG	3:C:8:GLU:N	2.02	0.73
2:B:81:ARG:NH1	4:B:161:HOH:O	2.08	0.73
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.37	0.73
2:E:74:GLU:OE2	4:E:150:HOH:O	2.07	0.73
1:A:121:LYS:HG3	2:B:1:ILE:HG13	1.70	0.72
1:A:177:GLU:OE1	4:A:411:HOH:O	2.07	0.72
2:E:54:LEU:HA	2:E:64:LEU:HD21	1.70	0.72
1:D:110:LEU:CA	4:D:369:HOH:O	2.38	0.71
1:D:154:GLU:OE1	4:D:346:HOH:O	2.08	0.71
2:E:91:LYS:HA	4:E:153:HOH:O	1.90	0.70
2:B:49:VAL:HG22	4:B:180:HOH:O	1.90	0.70
1:D:234:ARG:HE	1:D:242:GLN:HE21	1.39	0.69
1:D:216:THR:HG23	1:D:260:HIS:HB2	1.75	0.69
1:A:15:PRO:O	4:A:370:HOH:O	2.11	0.68
2:E:31:HIS:CA	4:E:145:HOH:O	2.42	0.68
1:D:110:LEU:O	4:D:369:HOH:O	2.12	0.68
1:D:249:VAL:HG21	1:D:254:GLU:HG3	1.75	0.68
2:B:54:LEU:HA	2:B:64:LEU:HD21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:GLN:NE2	4:C:103:HOH:O	2.26	0.67
1:A:20:PRO:O	4:A:315:HOH:O	2.12	0.66
1:D:181:ARG:HG3	4:D:403:HOH:O	1.94	0.66
1:A:109:PHE:CE2	4:A:423:HOH:O	2.50	0.65
1:A:131:ARG:NH1	4:A:416:HOH:O	2.27	0.65
3:F:7:LEU:HG	3:F:8:GLU:H	1.61	0.65
1:D:110:LEU:HG	4:D:369:HOH:O	1.97	0.65
2:E:88:SER:CB	4:E:147:HOH:O	2.43	0.64
1:D:110:LEU:CB	4:D:369:HOH:O	2.46	0.63
1:D:121:LYS:HG3	2:E:1:ILE:HG13	1.81	0.63
2:B:58:LYS:HE3	4:B:170:HOH:O	1.99	0.63
3:C:7:LEU:O	3:C:8:GLU:HB2	1.99	0.62
2:B:41:LYS:CA	4:B:183:HOH:O	2.24	0.62
4:A:397:HOH:O	2:B:99:MET:HA	1.99	0.62
1:A:204:TRP:CZ2	4:B:163:HOH:O	2.42	0.61
1:A:70:HIS:HD2	3:C:2:TYR:OH	1.83	0.60
4:A:397:HOH:O	2:B:99:MET:CA	2.50	0.60
1:A:220:ASP:O	4:A:424:HOH:O	2.16	0.60
1:D:274:TRP:N	4:D:372:HOH:O	2.35	0.59
2:E:5:PRO:HA	2:E:30:PHE:HB3	1.83	0.59
1:A:227:ASP:C	4:A:394:HOH:O	2.41	0.58
2:E:36:GLU:HG3	2:E:83:ASN:HB2	1.85	0.58
1:A:156:GLN:HE21	3:C:6:GLN:NE2	2.00	0.58
1:D:70:HIS:HD2	3:F:2:TYR:OH	1.87	0.58
1:D:19:GLU:HB3	1:D:75:ARG:HD2	1.86	0.57
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.40	0.57
2:E:1:ILE:HG21	2:E:3:ARG:HD2	1.87	0.57
1:D:170:ARG:HH22	3:F:1:LEU:HD21	1.68	0.57
2:E:7:ILE:HD12	2:E:91:LYS:HG2	1.85	0.56
3:C:7:LEU:O	3:C:8:GLU:CB	2.53	0.56
1:D:64:THR:O	1:D:68:LYS:HG3	2.06	0.56
3:C:7:LEU:CG	3:C:8:GLU:H	2.11	0.56
1:A:156:GLN:HE21	3:C:6:GLN:HE21	1.54	0.56
1:D:145:ARG:NH2	4:D:322:HOH:O	2.27	0.56
2:E:41[B]:LYS:HD2	2:E:46:ILE:HG12	1.87	0.55
2:E:58:LYS:H	2:E:58:LYS:HD2	1.70	0.55
1:A:49:ALA:O	1:A:52:ILE:HG22	2.05	0.55
1:D:258:THR:HG23	4:D:365:HOH:O	2.06	0.55
2:B:7:ILE:HD12	2:B:91:LYS:HG2	1.88	0.54
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.43	0.53
2:E:92:ILE:N	4:E:153:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:PRO:HD2	1:D:75:ARG:HD2	1.89	0.53
1:D:223:ASP:CA	4:D:374:HOH:O	2.56	0.53
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.92	0.53
1:A:64:THR:O	1:A:68:LYS:HG3	2.09	0.53
2:B:76:ASP:CB	4:B:156:HOH:O	2.57	0.53
1:A:234:ARG:HE	1:A:242:GLN:NE2	2.05	0.53
2:B:98:ASP:O	2:B:99:MET:HG3	2.08	0.52
1:D:49:ALA:O	1:D:52:ILE:HG22	2.08	0.52
1:A:124:ILE:HG13	4:A:421:HOH:O	2.08	0.52
1:D:213:ILE:HG12	1:D:214:THR:H	1.75	0.52
1:D:173:GLU:O	1:D:176:LYS:HB2	2.10	0.52
2:E:1:ILE:CG2	2:E:3:ARG:HD2	2.40	0.52
1:D:213:ILE:HG12	1:D:214:THR:N	2.25	0.52
2:E:41[B]:LYS:HD3	2:E:44:GLU:O	2.11	0.51
2:B:76:ASP:HB2	4:B:156:HOH:O	2.10	0.51
1:D:110:LEU:CG	4:D:369:HOH:O	2.53	0.51
3:C:6:GLN:CD	4:C:103:HOH:O	2.49	0.51
1:A:219:ARG:C	1:A:221:GLY:H	2.12	0.51
1:D:131:ARG:HH11	1:D:157:ARG:HH21	1.58	0.51
3:C:6:GLN:OE1	4:C:103:HOH:O	2.19	0.51
2:B:59:ASP:O	2:B:60:TRP:HB2	2.11	0.50
1:D:266:LEU:HD13	1:D:270:LEU:HG	1.94	0.50
3:F:7:LEU:O	3:F:8:GLU:CB	2.58	0.50
2:E:83:ASN:HD21	2:E:90:PRO:CG	2.21	0.50
2:B:83:ASN:HD21	2:B:90:PRO:CG	2.23	0.50
1:D:96:GLN:OE1	2:E:31:HIS:HE1	1.95	0.50
1:D:218:GLN:O	1:D:257:TYR:HA	2.13	0.49
1:A:127:LYS:HD2	1:A:132:SER:OG	2.13	0.49
2:B:68:THR:HG21	4:B:180:HOH:O	2.10	0.49
1:D:223:ASP:N	4:D:374:HOH:O	2.38	0.49
2:B:5:PRO:HA	2:B:30:PHE:HB3	1.95	0.48
1:D:218:GLN:HA	1:D:222:GLU:O	2.14	0.48
2:B:39:LEU:HD12	2:B:68:THR:HG22	1.96	0.48
1:A:244:TRP:CE2	4:A:397:HOH:O	2.54	0.47
2:E:59:ASP:O	2:E:60:TRP:HB2	2.14	0.47
1:D:68:LYS:O	1:D:71:SER:HB3	2.15	0.47
1:D:72:GLN:HE22	1:D:75:ARG:NH2	2.11	0.47
1:A:213:ILE:HG12	1:A:214:THR:N	2.30	0.47
1:A:143:THR:HG23	3:C:10:PHE:HA	1.96	0.47
1:A:76:GLU:O	1:A:80:ILE:HG13	2.14	0.47
1:A:121:LYS:HG3	2:B:1:ILE:CG1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ALA:HB3	4:D:334:HOH:O	2.14	0.47
1:D:111:ARG:NH1	4:D:373:HOH:O	2.48	0.47
1:D:29:ASP:OD2	4:D:358:HOH:O	2.21	0.46
2:E:31:HIS:N	4:E:145:HOH:O	2.48	0.46
1:A:72:GLN:HE22	1:A:75:ARG:CZ	2.27	0.46
2:B:31:HIS:CD2	2:B:32:PRO:HA	2.50	0.46
2:E:31:HIS:CD2	2:E:32:PRO:HA	2.51	0.46
1:D:146:LYS:HA	4:D:334:HOH:O	2.17	0.45
1:D:234:ARG:HE	1:D:242:GLN:NE2	2.09	0.45
1:A:157:ARG:NH2	4:A:335:HOH:O	2.37	0.45
1:D:82:LEU:CD2	1:D:87:GLN:HB2	2.47	0.45
2:E:38:ASP:HB3	2:E:45:ARG:HG2	1.99	0.45
1:A:8:PHE:HB3	2:B:56:PHE:CZ	2.52	0.45
2:B:38:ASP:OD1	2:B:45:ARG:HD3	2.16	0.45
2:E:3:ARG:HB2	4:E:145:HOH:O	2.16	0.44
2:E:31:HIS:C	4:E:145:HOH:O	2.43	0.44
2:B:58:LYS:H	2:B:58:LYS:HD2	1.83	0.44
1:D:40:ALA:HB3	4:D:304:HOH:O	2.18	0.44
2:E:5:PRO:CA	2:E:30:PHE:HB3	2.47	0.44
1:D:70:HIS:CD2	3:F:2:TYR:OH	2.67	0.44
1:A:43:GLN:N	4:A:386:HOH:O	2.45	0.44
2:B:19:LYS:HE2	4:B:157:HOH:O	2.18	0.44
2:E:41[B]:LYS:O	2:E:41[B]:LYS:HG2	2.18	0.43
1:A:5:MET:O	1:A:100:GLY:HA3	2.18	0.43
1:A:218:GLN:O	1:A:257:TYR:HA	2.17	0.43
1:A:233:THR:OG1	1:A:243:LYS:HD2	2.18	0.43
1:D:144:LYS:HE2	4:D:340:HOH:O	2.18	0.43
1:D:178:THR:O	1:D:181:ARG:HD2	2.18	0.43
1:A:192:HIS:HB3	4:A:409:HOH:O	2.18	0.43
1:A:218:GLN:HA	1:A:222:GLU:O	2.19	0.43
1:A:68:LYS:O	1:A:71:SER:HB3	2.19	0.42
1:D:127:LYS:HD2	1:D:132:SER:OG	2.19	0.42
2:B:5:PRO:CA	2:B:30:PHE:HB3	2.50	0.42
1:D:214:THR:HB	1:D:262:GLN:HB2	2.02	0.42
1:D:257:TYR:CE1	4:D:390:HOH:O	2.69	0.42
2:B:51:HIS:HD2	2:B:52:SER:O	2.03	0.42
1:A:212:GLU:HB3	4:A:355:HOH:O	2.19	0.42
2:B:70:PHE:CZ	2:B:72:PRO:HG3	2.55	0.41
2:B:98:ASP:O	4:B:163:HOH:O	2.21	0.41
1:D:35:ARG:HD3	2:E:53:ASP:OD2	2.20	0.41
1:D:58:GLU:HB3	4:D:376:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ARG:HH22	3:C:1:LEU:HD21	1.86	0.41
2:E:58:LYS:HD2	2:E:58:LYS:N	2.34	0.41
1:A:138:MET:HA	1:A:141:GLN:OE1	2.20	0.41
1:A:230:LEU:HD11	1:A:243:LYS:HE3	2.02	0.41
2:E:6:LYS:O	2:E:27:VAL:HA	2.20	0.41
1:D:131:ARG:NH1	1:D:157:ARG:NH2	2.68	0.41
2:E:40:LEU:O	2:E:78:TYR:HA	2.20	0.41
1:A:93:HIS:HD2	1:A:119:ASP:OD2	2.04	0.41
1:A:178:THR:CG2	4:A:396:HOH:O	2.69	0.41
2:B:58:LYS:N	2:B:58:LYS:HD2	2.35	0.41
1:A:219:ARG:C	1:A:221:GLY:N	2.74	0.41
1:A:266:LEU:HD13	1:A:270:LEU:HG	2.03	0.41
2:B:36:GLU:HB2	2:B:83:ASN:HB2	2.03	0.41
1:A:104:GLY:HA3	4:A:319:HOH:O	2.20	0.40
2:B:29:GLY:HA2	2:B:61:SER:OG	2.21	0.40
1:D:51:TRP:CE2	1:D:179:LEU:HD11	2.56	0.40
1:D:19:GLU:HA	1:D:20:PRO:HD3	1.85	0.40
1:D:170:ARG:NH2	3:F:1:LEU:HD21	2.35	0.40
1:A:192:HIS:HA	1:A:193:PRO:HD3	1.91	0.40
1:A:19:GLU:HG2	1:A:75:ARG:CZ	2.51	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)
4:A:430:HOH:O	4:B:186:HOH:O[2_545]	1.85	0.35

## 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	272/275 (99%)	257 (94%)	15 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	272/275 (99%)	262 (96%)	10 (4%)	0	100	100
2	B	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
2	E	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	18	26
3	C	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0	0
3	F	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0	0
All	All	755/770 (98%)	718 (95%)	34 (4%)	3 (0%)	38	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	8	GLU
3	F	8	GLU
2	E	47	GLU

### 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	230/231 (100%)	221 (96%)	9 (4%)	37	56
1	D	230/231 (100%)	220 (96%)	10 (4%)	33	52
2	B	94/95 (99%)	88 (94%)	6 (6%)	20	32
2	E	95/95 (100%)	89 (94%)	6 (6%)	21	33
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	8 (100%)	0	100	100
All	All	665/668 (100%)	634 (95%)	31 (5%)	30	48

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	134	THR
1	A	170	ARG

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Mol	Chain	Res	Type
1	A	180	GLN
1	A	181	ARG
1	A	197	HIS
1	A	216	THR
1	A	219	ARG
1	A	249	VAL
2	B	6	LYS
2	B	45	ARG
2	B	58	LYS
2	B	70	PHE
2	B	75	LYS
2	B	91	LYS
1	D	76	GLU
1	D	82	LEU
1	D	134	THR
1	D	157	ARG
1	D	170	ARG
1	D	180	GLN
1	D	181	ARG
1	D	194	ILE
1	D	216	THR
1	D	226	GLN
2	E	6	LYS
2	E	45	ARG
2	E	58	LYS
2	E	70	PHE
2	E	75	LYS
2	E	91	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	86	ASN
1	A	93	HIS
1	A	218	GLN
1	A	242	GLN
1	A	255	GLN
2	B	31	HIS
2	B	51	HIS
2	B	83	ASN
3	C	6	GLN

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Mol	Chain	Res	Type
1	D	70	HIS
1	D	86	ASN
1	D	93	HIS
1	D	115	GLN
1	D	192	HIS
1	D	218	GLN
1	D	242	GLN
1	D	255	GLN
2	E	31	HIS
2	E	51	HIS
2	E	83	ASN
3	F	6	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	274/275 (99%)	0.34	9 (3%) 47 45	9, 26, 51, 95	0
1	D	274/275 (99%)	0.47	17 (6%) 21 20	10, 31, 59, 95	0
2	B	99/100 (99%)	0.16	2 (2%) 65 63	10, 21, 44, 58	0
2	E	99/100 (99%)	0.21	1 (1%) 82 80	11, 23, 50, 60	0
3	C	10/10 (100%)	0.32	0 100 100	23, 31, 58, 60	0
3	F	10/10 (100%)	0.89	2 (20%) 1 1	30, 42, 87, 90	0
All	All	766/770 (99%)	0.35	31 (4%) 39 38	9, 27, 55, 95	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	HIS	4.0
1	D	225	THR	4.0
1	D	248	VAL	3.9
1	D	196	ASP	3.7
1	D	226	GLN	3.5
1	A	225	THR	3.3
1	D	251	SER	3.3
1	D	49	ALA	3.0
3	F	7	LEU	3.0
1	A	226	GLN	2.9
1	A	197	HIS	2.8
1	A	216	THR	2.8
1	D	253	GLU	2.7
1	D	228	THR	2.7
1	A	250	PRO	2.6
3	F	8	GLU	2.6
1	A	251	SER	2.6
1	D	195	SER	2.6
1	D	149	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	41[A]	LYS	2.5
1	D	230	LEU	2.4
1	D	1	GLY	2.4
1	D	131	ARG	2.3
1	A	136	ALA	2.3
2	B	99	MET	2.3
1	D	58	GLU	2.2
1	D	175	GLY	2.2
2	B	1	ILE	2.2
1	D	151	HIS	2.1
1	A	230	LEU	2.0
1	A	196	ASP	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.