



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:04 am GMT

PDB ID : 4WU5  
Title : HLA-A24 in complex with HIV-1 Nef134-8(wt)  
Authors : Shimizu, A.; Yamagata, A.; Fukai, S.; Iwamoto, A.  
Deposited on : 2014-10-31  
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

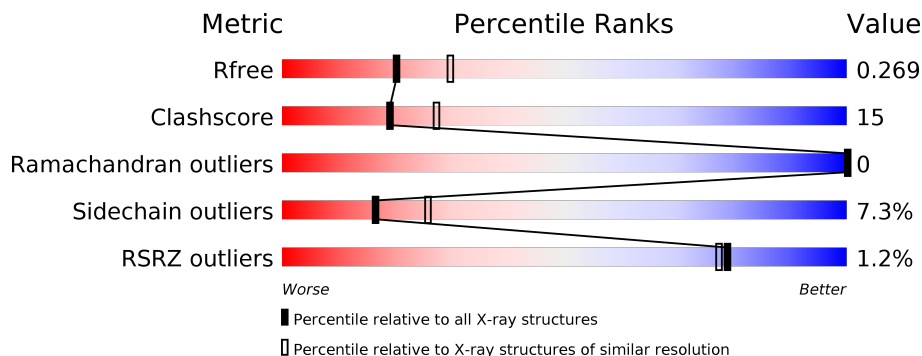
# 1 Overall quality at a glance

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>%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>.</div> </div> </div>
1	D	275	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>5%</div> </div> </div>
2	B	100	<div> <div></div> <div> <div></div> <div>65%</div> <div>30%</div> <div>.</div> </div> </div>
2	E	100	<div> <div></div> <div> <div></div> <div>62%</div> <div>33%</div> <div>.</div> </div> </div>
3	C	8	<div> <div></div> <div> <div></div> <div>88%</div> <div>13%</div> </div> </div>
3	F	8	<div> <div></div> <div> <div></div> <div>88%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6490 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	-	expression tag	UNP P05534
D	0	MET	-	expression tag	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	0	0
			829	528	140	158	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP P61769
E	0	MET	-	expression tag	UNP P61769

- Molecule 3 is a protein called 8-Mer peptide from Protein Nef.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			75	52	12	11			
3	F	8	Total	C	N	O	0	0	0
			75	52	12	11			

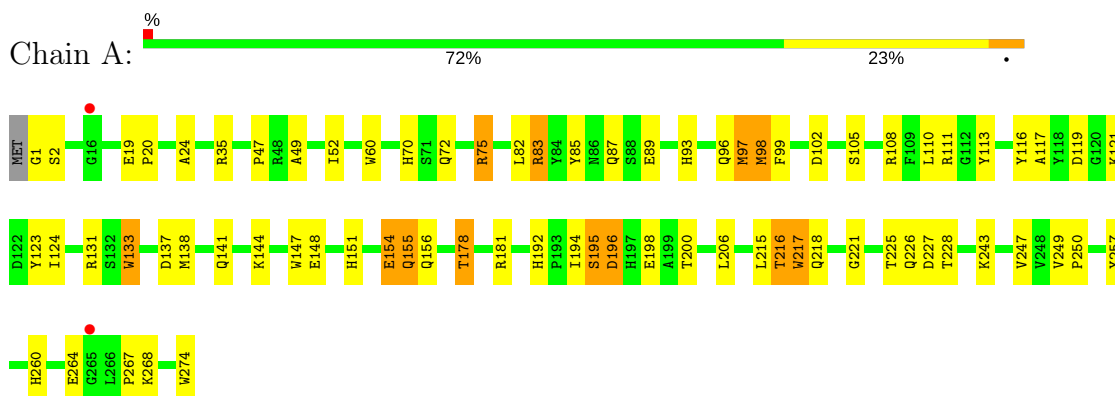
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total 89	O 89	0	0
4	B	36	Total 36	O 36	0	0
4	C	1	Total 1	O 1	0	0
4	D	81	Total 81	O 81	0	0
4	E	25	Total 25	O 25	0	0
4	F	6	Total 6	O 6	0	0

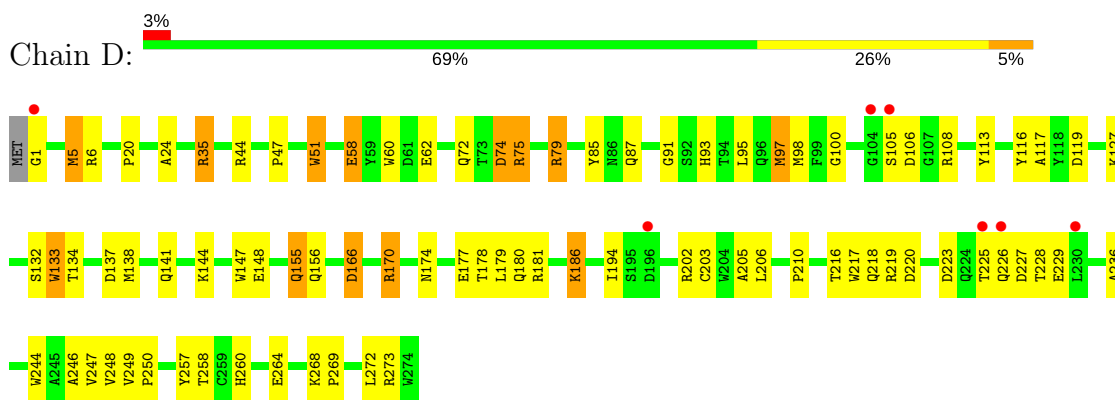
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

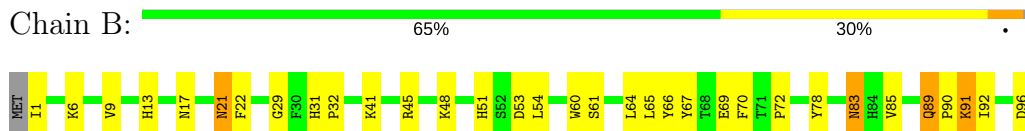
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain



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



- Molecule 2: Beta-2-microglobulin

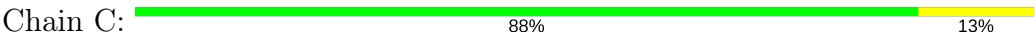


- Molecule 2: Beta-2-microglobulin

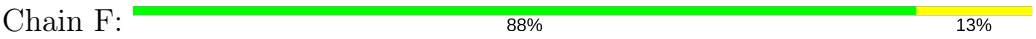




- Molecule 3: 8-Mer peptide from Protein Nef



- Molecule 3: 8-Mer peptide from Protein Nef



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.69Å 67.07Å 117.73Å 90.00° 99.01° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 43.42 – 2.37	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.40) 96.3 (43.42-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.37Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.231 , 0.271 0.230 , 0.269	Depositor DCC
$R_{free}$ test set	1712 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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 24.04 % 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 4.1440e-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	0.57	4/2282 (0.2%)	0.53	0/3092
1	D	0.57	4/2282 (0.2%)	0.52	0/3092
2	B	0.53	0/852	0.51	0/1152
2	E	0.55	1/852 (0.1%)	0.52	0/1152
3	C	0.82	0/79	0.69	0/106
3	F	0.80	0/79	0.63	0/106
All	All	0.57	9/6426 (0.1%)	0.53	0/8700

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	TRP	CD2-CE2	5.16	1.47	1.41
1	D	147	TRP	CD2-CE2	5.15	1.47	1.41
1	D	133	TRP	CD2-CE2	5.09	1.47	1.41
1	A	147	TRP	CD2-CE2	5.08	1.47	1.41
1	A	274	TRP	CD2-CE2	5.08	1.47	1.41
1	D	51	TRP	CD2-CE2	5.06	1.47	1.41
1	A	133	TRP	CD2-CE2	5.01	1.47	1.41
2	E	60	TRP	CD2-CE2	5.01	1.47	1.41
1	D	244	TRP	CD2-CE2	5.00	1.47	1.41

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	58	0
1	D	2222	0	2082	71	0
2	B	829	0	794	28	0
2	E	829	0	794	28	0
3	C	75	0	71	5	0
3	F	75	0	71	6	0
4	A	89	0	0	4	0
4	B	36	0	0	0	0
4	C	1	0	0	0	0
4	D	81	0	0	9	0
4	E	25	0	0	3	0
4	F	6	0	0	1	0
All	All	6490	0	5894	177	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 15.

All (177) 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)
2:E:21:ASN:ND2	2:E:22:PHE:H	1.39	1.19
2:E:21:ASN:HD22	2:E:22:PHE:N	1.40	1.18
1:A:228:THR:HG22	1:A:247:VAL:HG12	1.45	0.99
1:D:166:ASP:HB3	4:D:344:HOH:O	1.63	0.98
1:D:228:THR:HG22	1:D:247:VAL:HG12	1.42	0.98
2:E:85:VAL:HB	4:E:120:HOH:O	1.61	0.97
2:B:91:LYS:HZ2	2:B:92:ILE:H	0.97	0.93
2:B:21:ASN:HD22	2:B:22:PHE:H	1.10	0.90
2:B:21:ASN:ND2	2:B:22:PHE:H	1.70	0.89
1:A:72:GLN:HE22	1:A:75:ARG:HH21	1.21	0.88
2:B:21:ASN:HD22	2:B:22:PHE:N	1.76	0.83
1:D:97:MET:CE	3:F:5:THR:HG22	2.09	0.83
1:D:138:MET:HA	1:D:141:GLN:HG3	1.58	0.83
1:A:192:HIS:HD2	4:A:379:HOH:O	1.62	0.82
1:A:138:MET:HA	1:A:141:GLN:HG3	1.61	0.80
2:B:91:LYS:HZ2	2:B:92:ILE:N	1.79	0.80
1:A:215:LEU:HD12	1:A:243:LYS:HD3	1.64	0.79
1:A:97:MET:CE	3:C:5:THR:HG22	2.13	0.78
1:D:74:ASP:OD2	1:D:95:LEU:HD22	1.82	0.78
1:D:97:MET:CE	3:F:5:THR:CG2	2.61	0.78
1:D:97:MET:HE1	3:F:5:THR:CG2	2.17	0.74
2:E:85:VAL:HG23	4:E:108:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:MET:HE1	3:C:5:THR:CG2	2.19	0.72
1:D:58:GLU:O	1:D:62:GLU:HG3	1.90	0.70
1:A:20:PRO:HD2	1:A:75:ARG:HD3	1.72	0.70
1:D:72:GLN:HE22	1:D:75:ARG:NH2	1.90	0.69
2:B:91:LYS:NZ	2:B:92:ILE:H	1.85	0.68
1:D:170:ARG:HD3	1:D:174:ASN:HD21	1.59	0.68
2:E:99:MET:HE3	4:E:115:HOH:O	1.94	0.67
2:E:51:HIS:HD2	2:E:52:SER:O	1.77	0.67
1:D:97:MET:HG3	1:D:116:TYR:CE2	2.30	0.67
1:D:258:THR:HG23	1:D:260:HIS:NE2	2.09	0.66
1:A:97:MET:HE1	3:C:5:THR:HG22	1.77	0.66
1:D:138:MET:CE	1:D:141:GLN:HE21	2.08	0.66
2:B:13:HIS:H	2:B:21:ASN:HD21	1.44	0.65
1:A:108:ARG:HH12	1:D:91:GLY:HA2	1.62	0.65
1:D:219:ARG:HG2	4:D:340:HOH:O	1.97	0.64
2:E:31:HIS:CD2	2:E:32:PRO:HA	2.32	0.64
1:A:72:GLN:NE2	1:A:75:ARG:HH21	1.93	0.64
1:A:151:HIS:O	1:A:154:GLU:HG2	1.98	0.63
1:A:228:THR:HG22	1:A:247:VAL:CG1	2.26	0.62
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.34	0.62
2:E:91:LYS:HA	2:E:91:LYS:NZ	2.14	0.62
1:A:108:ARG:NH1	1:D:91:GLY:HA2	2.14	0.62
1:D:137:ASP:O	1:D:141:GLN:HG2	2.00	0.61
2:B:1:ILE:HG13	2:B:1:ILE:O	1.99	0.61
1:D:85:TYR:HB2	1:D:87:GLN:HG3	1.81	0.61
1:D:273:ARG:NH1	1:D:273:ARG:HB2	2.16	0.60
1:A:178:THR:O	1:A:181:ARG:HG2	2.01	0.60
1:A:97:MET:CE	3:C:5:THR:CG2	2.78	0.59
1:A:47:PRO:HB3	1:A:60:TRP:CH2	2.38	0.59
1:D:97:MET:HE2	3:F:5:THR:HG22	1.85	0.59
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.36	0.59
1:D:79:ARG:HG3	1:D:79:ARG:HH11	1.67	0.59
1:A:20:PRO:HD2	1:A:75:ARG:HH11	1.67	0.58
2:E:21:ASN:HD22	2:E:22:PHE:H	0.66	0.58
1:D:180:GLN:O	1:D:180:GLN:HG3	2.02	0.58
1:D:24:ALA:O	1:D:35:ARG:HA	2.04	0.58
2:B:91:LYS:HA	2:B:91:LYS:NZ	2.20	0.57
1:D:228:THR:HG22	1:D:247:VAL:CG1	2.26	0.57
1:A:98:MET:HE3	1:A:99:PHE:N	2.20	0.57
1:D:155:GLN:HG3	1:D:156:GLN:N	2.20	0.57
1:D:268:LYS:HG3	1:D:269:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LYS:O	1:A:148:GLU:HG3	2.05	0.56
1:A:206:LEU:HD12	4:A:303:HOH:O	2.05	0.56
1:A:144:LYS:HE2	1:A:148:GLU:OE2	2.05	0.56
1:A:98:MET:HE1	1:A:113:TYR:HB2	1.86	0.56
2:B:91:LYS:HA	2:B:91:LYS:HZ3	1.70	0.56
1:D:106:ASP:OD2	1:D:108:ARG:HD2	2.05	0.56
1:A:155:GLN:HG3	1:A:156:GLN:N	2.20	0.56
1:A:226:GLN:HG2	1:A:227:ASP:H	1.71	0.56
1:A:72:GLN:HE22	1:A:75:ARG:NH2	1.98	0.56
1:D:20:PRO:HD2	1:D:75:ARG:HD3	1.87	0.55
2:E:96:ASP:HB3	2:E:99:MET:HA	1.89	0.55
1:D:170:ARG:HD2	4:F:105:HOH:O	2.06	0.55
1:A:196:ASP:OD1	1:A:196:ASP:N	2.39	0.55
1:A:200:THR:HG23	4:A:352:HOH:O	2.07	0.55
1:D:170:ARG:NH1	4:D:351:HOH:O	2.40	0.55
1:D:202:ARG:HG3	1:D:246:ALA:HB2	1.89	0.55
1:D:93:HIS:HD2	1:D:119:ASP:OD2	1.90	0.54
1:D:133:TRP:O	1:D:144:LYS:NZ	2.40	0.54
1:D:180:GLN:HB2	4:D:368:HOH:O	2.06	0.54
1:A:70:HIS:CD2	3:C:5:THR:HG21	2.43	0.54
2:E:59:ASP:O	2:E:60:TRP:HB2	2.09	0.53
1:A:72:GLN:NE2	1:A:75:ARG:NH2	2.56	0.53
2:B:70:PHE:CE2	2:B:72:PRO:HG3	2.44	0.53
1:D:58:GLU:HA	4:D:358:HOH:O	2.08	0.53
2:B:54:LEU:HA	2:B:64:LEU:HD21	1.91	0.53
1:D:236:ALA:HB1	2:E:12:ARG:HG3	1.90	0.53
2:E:24:ASN:HB3	2:E:65:LEU:HD11	1.91	0.53
1:D:249:VAL:HG12	1:D:250:PRO:O	2.09	0.52
1:A:131:ARG:HH12	2:E:38:ASP:CG	2.13	0.52
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.92	0.52
1:A:218:GLN:NE2	1:A:221:GLY:HA2	2.24	0.52
1:A:102:ASP:OD2	1:A:111:ARG:NH1	2.43	0.51
1:D:51:TRP:CZ2	1:D:179:LEU:HD11	2.45	0.51
1:A:83:ARG:HG2	1:A:83:ARG:HH11	1.76	0.51
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.93	0.51
1:A:97:MET:HG3	1:A:116:TYR:CE2	2.45	0.51
2:B:29:GLY:HA2	2:B:61:SER:OG	2.11	0.51
1:A:123:TYR:HD2	1:A:124:ILE:HG22	1.76	0.50
1:D:218:GLN:HB2	1:D:258:THR:HG23	1.94	0.50
1:A:82:LEU:HD13	1:A:89:GLU:HG2	1.93	0.50
2:E:54:LEU:HA	2:E:64:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ASP:HB3	2:B:99:MET:HA	1.94	0.50
2:E:91:LYS:HA	2:E:91:LYS:HZ2	1.77	0.50
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.95	0.49
1:D:186:LYS:H	1:D:186:LYS:HE2	1.78	0.49
1:A:226:GLN:HG2	1:A:227:ASP:N	2.27	0.49
2:B:96:ASP:O	2:B:99:MET:HG3	2.13	0.49
1:D:226:GLN:HG3	1:D:227:ASP:H	1.77	0.49
1:D:226:GLN:HG3	1:D:227:ASP:N	2.26	0.49
2:E:1:ILE:HG13	2:E:1:ILE:O	2.13	0.49
1:A:249:VAL:HG13	1:A:257:TYR:CE1	2.48	0.48
1:D:264:GLU:HA	4:D:333:HOH:O	2.13	0.48
2:B:9:VAL:HG13	2:B:9:VAL:O	2.13	0.48
2:E:42:ASN:HA	2:E:77:GLU:OE2	2.13	0.48
1:D:181:ARG:HH11	1:D:181:ARG:HG2	1.79	0.48
1:D:144:LYS:HE2	4:D:375:HOH:O	2.14	0.47
1:A:137:ASP:O	1:A:141:GLN:HG2	2.15	0.47
1:A:267:PRO:HB2	1:A:268:LYS:HD2	1.97	0.47
1:D:229:GLU:HB3	4:D:353:HOH:O	2.14	0.47
1:A:1:GLY:O	1:A:105:SER:HA	2.14	0.46
1:A:264:GLU:HG2	4:A:342:HOH:O	2.14	0.46
1:D:273:ARG:HB2	1:D:273:ARG:HH11	1.80	0.46
1:A:216:THR:HG23	1:A:260:HIS:HB2	1.96	0.46
1:A:49:ALA:O	1:A:52:ILE:HG22	2.16	0.46
1:A:35:ARG:HD3	2:B:53:ASP:OD2	2.16	0.46
1:A:195:SER:OG	1:A:196:ASP:N	2.48	0.45
2:E:21:ASN:ND2	2:E:22:PHE:N	2.21	0.45
1:D:138:MET:CE	1:D:141:GLN:NE2	2.78	0.45
1:A:24:ALA:O	1:A:35:ARG:HA	2.16	0.45
2:B:51:HIS:HB3	2:B:66:TYR:CD2	2.50	0.45
1:D:273:ARG:CB	1:D:273:ARG:HH11	2.28	0.45
1:A:19:GLU:OE1	1:A:75:ARG:HD2	2.17	0.45
1:D:205:ALA:O	1:D:206:LEU:HD23	2.16	0.45
1:D:1:GLY:O	1:D:105:SER:HA	2.16	0.44
1:D:97:MET:HE1	3:F:5:THR:HG21	1.95	0.44
2:E:2:GLN:HG2	2:E:86:THR:HG22	1.99	0.44
2:B:51:HIS:HA	2:B:65:LEU:O	2.18	0.44
1:A:217:TRP:CD1	1:A:247:VAL:HG13	2.52	0.44
2:B:54:LEU:HA	2:B:64:LEU:CD2	2.48	0.44
2:E:10:TYR:N	2:E:10:TYR:CD1	2.86	0.44
1:D:44:ARG:HB3	1:D:44:ARG:NH1	2.33	0.44
1:A:98:MET:HE3	1:A:98:MET:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:PRO:HB3	2:E:30:PHE:HB3	2.00	0.43
1:D:194:ILE:HD11	1:D:248:VAL:HG13	1.99	0.43
1:D:97:MET:CE	3:F:5:THR:HG21	2.44	0.43
2:B:67:TYR:CD1	2:B:67:TYR:N	2.87	0.43
1:D:79:ARG:HG2	1:D:79:ARG:H	1.72	0.43
1:A:249:VAL:HG12	1:A:250:PRO:O	2.19	0.43
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.54	0.43
1:D:97:MET:HG3	1:D:116:TYR:CZ	2.54	0.43
1:D:177:GLU:HG2	1:D:178:THR:N	2.34	0.43
1:D:47:PRO:HB3	1:D:60:TRP:CH2	2.54	0.42
1:D:5:MET:O	1:D:100:GLY:HA3	2.18	0.42
1:D:218:GLN:HB2	1:D:258:THR:CG2	2.48	0.42
1:D:258:THR:CG2	1:D:260:HIS:NE2	2.81	0.42
2:B:41:LYS:HE3	2:B:78:TYR:OH	2.19	0.42
1:A:194:ILE:HG12	1:A:198:GLU:O	2.19	0.42
1:D:132:SER:HB2	4:D:380:HOH:O	2.19	0.42
2:E:96:ASP:O	2:E:99:MET:HG2	2.19	0.41
1:D:6:ARG:NH2	1:D:113:TYR:CE1	2.88	0.41
1:D:127:LYS:HE2	1:D:134:THR:OG1	2.19	0.41
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.55	0.41
2:E:71:THR:HA	2:E:72:PRO:HD2	1.93	0.41
1:A:85:TYR:HB2	1:A:87:GLN:HG3	2.01	0.41
2:B:31:HIS:CD2	2:B:32:PRO:HA	2.55	0.41
1:D:272:LEU:HD12	1:D:272:LEU:N	2.35	0.41
2:B:89:GLN:O	2:B:90:PRO:C	2.59	0.41
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.55	0.41
2:E:23:LEU:O	2:E:67:TYR:HA	2.21	0.41
1:D:210:PRO:HG2	1:D:264:GLU:OE2	2.20	0.41
2:B:83:ASN:HD22	2:B:83:ASN:HA	1.64	0.41
1:D:144:LYS:O	1:D:148:GLU:HG3	2.21	0.41
2:E:51:HIS:CD2	2:E:52:SER:O	2.65	0.41
2:E:89:GLN:O	2:E:90:PRO:C	2.59	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	272/275 (99%)	265 (97%)	7 (3%)	0	100	100
1	D	272/275 (99%)	263 (97%)	9 (3%)	0	100	100
2	B	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
2	E	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	F	6/8 (75%)	6 (100%)	0	0	100	100
All	All	750/766 (98%)	728 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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%)	216 (94%)	14 (6%)	22	34
1	D	230/231 (100%)	214 (93%)	16 (7%)	18	28
2	B	94/95 (99%)	84 (89%)	10 (11%)	8	11
2	E	94/95 (99%)	86 (92%)	8 (8%)	12	19
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
All	All	662/666 (99%)	614 (93%)	48 (7%)	16	26

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	75	ARG
1	A	83	ARG

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Mol	Chain	Res	Type
1	A	97	MET
1	A	98	MET
1	A	110	LEU
1	A	121	LYS
1	A	154	GLU
1	A	155	GLN
1	A	178	THR
1	A	195	SER
1	A	196	ASP
1	A	216	THR
1	A	225	THR
2	B	6	LYS
2	B	17	ASN
2	B	21	ASN
2	B	45	ARG
2	B	48	LYS
2	B	69	GLU
2	B	83	ASN
2	B	85	VAL
2	B	89	GLN
2	B	91	LYS
1	D	5	MET
1	D	35	ARG
1	D	58	GLU
1	D	74	ASP
1	D	75	ARG
1	D	79	ARG
1	D	97	MET
1	D	98	MET
1	D	155	GLN
1	D	166	ASP
1	D	170	ARG
1	D	186	LYS
1	D	216	THR
1	D	220	ASP
1	D	223	ASP
1	D	225	THR
2	E	21	ASN
2	E	48	LYS
2	E	70	PHE
2	E	75	LYS
2	E	77	GLU

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Mol	Chain	Res	Type
2	E	83	ASN
2	E	91	LYS
2	E	98	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	86	ASN
1	A	93	HIS
1	A	155	GLN
1	A	180	GLN
1	A	218	GLN
1	A	255	GLN
2	B	21	ASN
2	B	31	HIS
2	B	83	ASN
1	D	72	GLN
1	D	86	ASN
1	D	93	HIS
1	D	141	GLN
1	D	151	HIS
1	D	155	GLN
1	D	174	ASN
1	D	218	GLN
2	E	13	HIS
2	E	21	ASN
2	E	31	HIS
2	E	51	HIS
2	E	83	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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 [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, 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%)	-0.23	2 (0%) 87 86	19, 31, 51, 69	0
1	D	274/275 (99%)	-0.04	7 (2%) 56 54	19, 32, 52, 82	0
2	B	99/100 (99%)	-0.14	0 100 100	21, 36, 57, 65	0
2	E	99/100 (99%)	-0.09	0 100 100	23, 34, 53, 61	0
3	C	8/8 (100%)	-0.16	0 100 100	20, 22, 27, 31	0
3	F	8/8 (100%)	0.04	0 100 100	25, 29, 31, 42	0
All	All	762/766 (99%)	-0.13	9 (1%) 79 77	19, 32, 52, 82	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	225	THR	3.8
1	D	226	GLN	3.1
1	A	265	GLY	2.8
1	D	1	GLY	2.8
1	D	104	GLY	2.6
1	D	105	SER	2.4
1	A	16	GLY	2.4
1	D	196	ASP	2.3
1	D	230	LEU	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.