



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 08:52 PM BST

PDB ID : 6VR1  
Title : Complex of HLA-A2, a class I MHC, with a p53 peptide  
Authors : Wu, D.; Pierce, B.G.; Gallagher, D.T.; Mariuzza, R.A.  
Deposited on : 2020-02-06  
Resolution : 2.37 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

<https://www.wwpdb.org/validation/2017/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) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

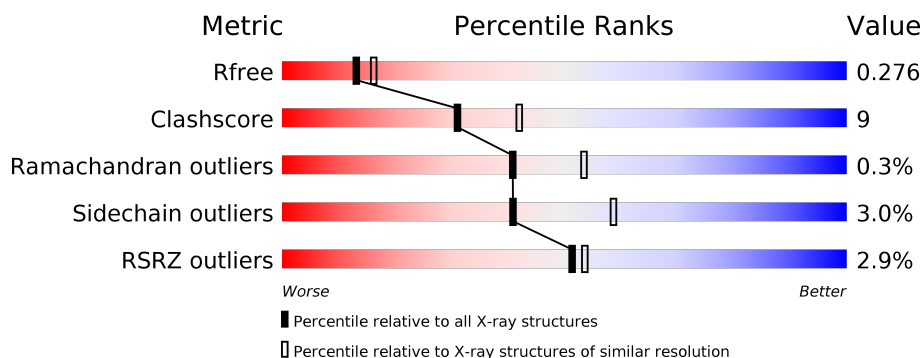
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	293	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>6%</div> </div> </div>
1	D	293	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>6%</div> </div> </div>
2	B	100	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>
2	E	100	<div> <div></div> <div> <div></div> <div>79%</div> <div>21%</div> </div> </div>
3	P	9	<div> <div></div> <div> <div></div> <div>56%</div> <div>44%</div> </div> </div>
3	Q	9	<div> <div></div> <div> <div></div> <div>33%</div> <div>67%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6514 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2219	1389	402	419	9			
1	D	275	Total	C	N	O	S	0	0	0
			2184	1371	388	416	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q861F7
A	276	GLY	-	expression tag	UNP Q861F7
A	277	GLY	-	expression tag	UNP Q861F7
A	278	GLY	-	expression tag	UNP Q861F7
A	279	LEU	-	expression tag	UNP Q861F7
A	280	ASN	-	expression tag	UNP Q861F7
A	281	ASP	-	expression tag	UNP Q861F7
A	282	ILE	-	expression tag	UNP Q861F7
A	283	PHE	-	expression tag	UNP Q861F7
A	284	GLU	-	expression tag	UNP Q861F7
A	285	ALA	-	expression tag	UNP Q861F7
A	286	GLN	-	expression tag	UNP Q861F7
A	287	LYS	-	expression tag	UNP Q861F7
A	288	ILE	-	expression tag	UNP Q861F7
A	289	GLU	-	expression tag	UNP Q861F7
A	290	TRP	-	expression tag	UNP Q861F7
A	291	HIS	-	expression tag	UNP Q861F7
A	292	GLU	-	expression tag	UNP Q861F7
D	0	MET	-	initiating methionine	UNP Q861F7
D	276	GLY	-	expression tag	UNP Q861F7
D	277	GLY	-	expression tag	UNP Q861F7
D	278	GLY	-	expression tag	UNP Q861F7
D	279	LEU	-	expression tag	UNP Q861F7
D	280	ASN	-	expression tag	UNP Q861F7
D	281	ASP	-	expression tag	UNP Q861F7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	282	ILE	-	expression tag	UNP Q861F7
D	283	PHE	-	expression tag	UNP Q861F7
D	284	GLU	-	expression tag	UNP Q861F7
D	285	ALA	-	expression tag	UNP Q861F7
D	286	GLN	-	expression tag	UNP Q861F7
D	287	LYS	-	expression tag	UNP Q861F7
D	288	ILE	-	expression tag	UNP Q861F7
D	289	GLU	-	expression tag	UNP Q861F7
D	290	TRP	-	expression tag	UNP Q861F7
D	291	HIS	-	expression tag	UNP Q861F7
D	292	GLU	-	expression tag	UNP Q861F7

- 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
			801	511	137	150	3			
2	E	100	Total	C	N	O	S	0	0	0
			806	516	137	149	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P61769
E	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Cellular tumor antigen p53 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	S	0	0	0
			77	45	17	13	2			
3	Q	9	Total	C	N	O	S	0	0	0
			77	45	17	13	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	28	Total	O	0	0
			28	28		

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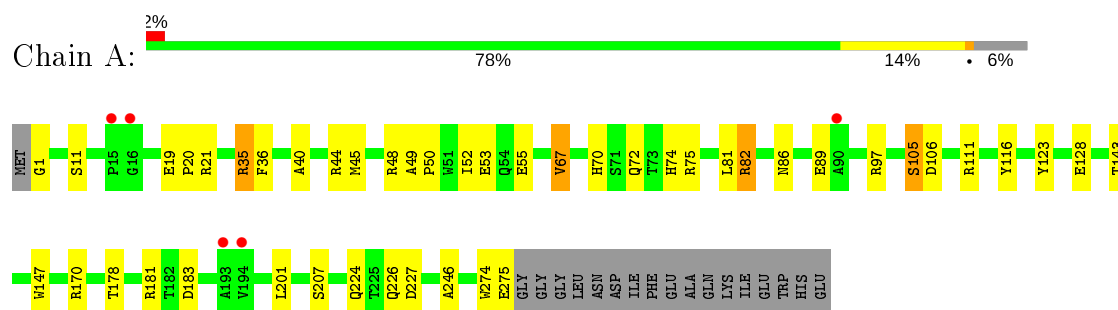
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	95	Total 95	O 95	0	0
4	E	52	Total 52	O 52	0	0
4	P	10	Total 10	O 10	0	0
4	Q	4	Total 4	O 4	0	0

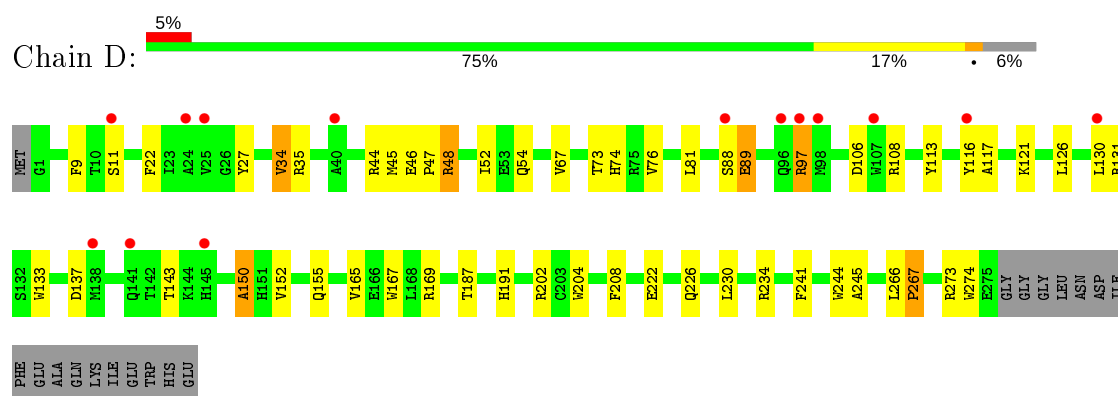
### 3 Residue-property plots [i](#)

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

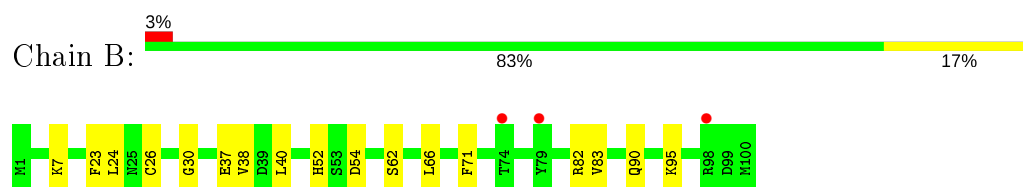
#### • Molecule 1: MHC class I antigen



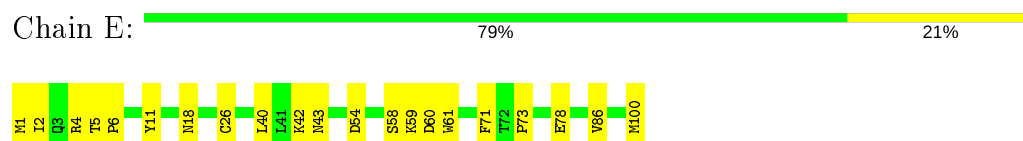
#### • Molecule 1: MHC class I antigen



#### • Molecule 2: Beta-2-microglobulin

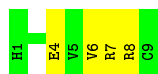


#### • Molecule 2: Beta-2-microglobulin



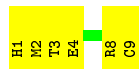
- Molecule 3: Cellular tumor antigen p53 peptide

Chain P:  56% 44%



- Molecule 3: Cellular tumor antigen p53 peptide

Chain Q:  33% 67%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.33Å 79.73Å 85.85Å 90.00° 101.68° 90.00°	Depositor
Resolution (Å)	20.00 – 2.37 39.75 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.37) 99.8 (39.75-2.37)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.217 , 0.274 0.217 , 0.276	Depositor DCC
$R_{free}$ test set	1879 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 48.9	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	0.93	EDS
Total number of atoms	6514	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<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	0.63	0/2283	1.05	3/3102 (0.1%)
1	D	0.63	2/2249 (0.1%)	1.02	3/3064 (0.1%)
2	B	0.53	0/824	0.92	0/1123
2	E	0.60	0/829	0.98	0/1127
3	P	0.85	0/77	1.56	1/100 (1.0%)
3	Q	0.59	0/77	0.88	0/100
All	All	0.62	2/6339 (0.0%)	1.02	7/8616 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	97	ARG	N-CA	-11.76	1.22	1.46
1	D	150	ALA	CA-CB	-7.48	1.36	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ARG	CG-CD-NE	-6.70	97.73	111.80
1	A	21	ARG	CG-CD-NE	5.52	123.38	111.80
1	A	35	ARG	CG-CD-NE	5.43	123.21	111.80
3	P	7	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	D	273	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	97	ARG	CB-CA-C	5.08	120.57	110.40
1	D	27	TYR	CB-CA-C	-5.07	100.25	110.40

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	2219	0	2060	32	0
1	D	2184	0	1990	54	0
2	B	801	0	736	12	0
2	E	806	0	752	13	0
3	P	77	0	80	1	0
3	Q	77	0	80	12	0
4	A	161	0	0	6	1
4	B	28	0	0	1	0
4	D	95	0	0	7	2
4	E	52	0	0	2	0
4	P	10	0	0	1	1
4	Q	4	0	0	0	0
All	All	6514	0	5698	108	2

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 9.

All (108) 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:208:PHE:O	4:D:302:HOH:O	1.67	1.13
2:E:60:ASP:O	4:E:201:HOH:O	2.00	0.80
1:D:241:PHE:HD2	4:D:302:HOH:O	1.68	0.77
1:D:73:THR:HG23	3:Q:8:ARG:HD3	1.67	0.76
1:A:178:THR:HG21	4:A:353:HOH:O	1.86	0.74
1:A:35:ARG:HH11	1:A:48:ARG:HH21	1.35	0.74
1:D:165:VAL:O	1:D:169:ARG:HG3	1.89	0.72
1:A:35:ARG:NH1	4:A:302:HOH:O	2.23	0.71
1:A:35:ARG:NH1	1:A:48:ARG:HH21	1.89	0.70
1:A:181:ARG:NH1	1:A:183:ASP:OD2	2.26	0.69
1:D:117:ALA:HB2	2:E:61:TRP:CE2	2.27	0.69
1:D:67:VAL:HB	3:Q:2:MET:HE3	1.75	0.69
1:D:226:GLN:NE2	4:D:303:HOH:O	2.27	0.68
1:A:1:GLY:O	1:A:105:SER:HA	1.94	0.67
1:D:81:LEU:HD11	3:Q:9:CYS:SG	2.34	0.67
1:D:67:VAL:HB	3:Q:2:MET:CE	2.24	0.66
1:A:227:ASP:OD2	4:A:301:HOH:O	2.13	0.66
2:B:30:GLY:HA2	2:B:62:SER:OG	1.96	0.66
3:P:4:GLU:OE2	4:P:101:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:GLN:HB3	4:B:219:HOH:O	1.98	0.64
1:D:48:ARG:HG2	1:D:48:ARG:NH1	2.12	0.64
1:D:97:ARG:NH1	1:D:116:TYR:HE1	1.96	0.64
4:A:427:HOH:O	1:D:155:GLN:HG2	1.97	0.64
1:D:35:ARG:HH11	1:D:48:ARG:HH21	1.46	0.62
2:E:18:ASN:HA	2:E:73:PRO:O	1.99	0.62
1:A:35:ARG:HD3	1:A:48:ARG:NH2	2.17	0.59
1:A:86:ASN:ND2	4:A:307:HOH:O	2.33	0.59
1:D:48:ARG:HH11	1:D:48:ARG:HG2	1.70	0.57
1:A:35:ARG:HD2	2:B:54:ASP:OD2	2.06	0.56
1:D:117:ALA:HB2	2:E:61:TRP:CD2	2.41	0.56
1:D:234:ARG:HH12	2:E:100:MET:CE	2.19	0.55
1:D:230:LEU:HD12	1:D:245:ALA:HB2	1.87	0.55
1:D:106:ASP:CG	1:D:108:ARG:HG3	2.27	0.55
1:A:111:ARG:CZ	1:A:128:GLU:OE2	2.55	0.54
1:A:20:PRO:HG2	1:A:75:ARG:HG3	1.90	0.53
1:D:81:LEU:CD1	3:Q:9:CYS:SG	2.97	0.53
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.44	0.53
1:D:35:ARG:HD2	2:E:54:ASP:OD2	2.09	0.52
1:D:34:VAL:HG13	1:D:45:MET:HE3	1.91	0.52
1:A:70:HIS:CD2	1:A:97:ARG:HH21	2.27	0.52
1:D:191:HIS:HB2	1:D:274:TRP:CZ2	2.43	0.52
1:A:116:TYR:CE2	1:A:147:TRP:HH2	2.29	0.51
1:A:49:ALA:O	1:A:52:ILE:HG22	2.11	0.51
2:B:23:PHE:C	2:B:71:PHE:HE1	2.14	0.51
1:D:241:PHE:CD2	4:D:302:HOH:O	2.52	0.50
1:D:167:TRP:CG	3:Q:1:HIS:HB2	2.47	0.50
1:D:34:VAL:HG13	1:D:45:MET:CE	2.41	0.50
1:D:150:ALA:HB3	1:D:152:VAL:HG23	1.94	0.50
1:A:97:ARG:HD3	1:A:116:TYR:CZ	2.46	0.50
2:B:24:LEU:HB2	2:B:71:PHE:CE1	2.47	0.50
1:D:126:LEU:HD13	1:D:133:TRP:CH2	2.46	0.50
1:D:74:HIS:NE2	1:D:97:ARG:HD2	2.27	0.50
1:D:76:VAL:HG21	3:Q:8:ARG:NH1	2.28	0.49
1:A:201:LEU:O	1:A:246:ALA:HA	2.11	0.49
2:E:2:ILE:HG21	2:E:4:ARG:NH1	2.28	0.49
1:D:241:PHE:N	4:D:302:HOH:O	2.46	0.48
2:B:24:LEU:N	2:B:71:PHE:CE1	2.81	0.48
2:B:24:LEU:N	2:B:71:PHE:HE1	2.11	0.48
1:D:88:SER:O	1:D:89:GLU:HB2	2.13	0.48
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:NH1	1:D:48:ARG:HH21	2.12	0.47
1:A:55:GLU:OE1	1:A:170:ARG:NH2	2.47	0.47
2:B:52:HIS:HA	2:B:66:LEU:O	2.14	0.47
1:D:44:ARG:O	1:D:46:GLU:HG3	2.15	0.47
1:D:137:ASP:OD1	1:D:137:ASP:C	2.53	0.47
1:A:224:GLN:NE2	1:A:226:GLN:O	2.48	0.47
1:A:11:SER:OG	1:A:74:HIS:HB3	2.15	0.47
2:E:58:SER:O	2:E:59:LYS:C	2.52	0.47
1:D:191:HIS:HB2	1:D:274:TRP:CH2	2.49	0.46
1:A:50:PRO:O	1:A:53:GLU:HG3	2.16	0.46
2:B:37:GLU:O	2:B:83:VAL:HA	2.15	0.46
1:A:82:ARG:CZ	1:A:89:GLU:HG2	2.46	0.46
2:B:26:CYS:HB2	2:B:40:LEU:HD21	1.97	0.46
2:E:11:TYR:N	2:E:11:TYR:CD1	2.84	0.46
1:A:40:ALA:HB3	4:A:327:HOH:O	2.16	0.46
2:E:5:THR:OG1	2:E:6:PRO:HD2	2.16	0.46
1:A:35:ARG:HH11	1:A:48:ARG:NH2	2.09	0.45
1:A:36:PHE:CD2	1:A:67:VAL:HG11	2.51	0.45
1:A:35:ARG:NH1	1:A:48:ARG:NH2	2.62	0.45
1:A:274:TRP:O	1:A:275:GLU:HB2	2.16	0.45
1:A:123:TYR:HH	1:A:143:THR:HG1	1.64	0.45
1:A:35:ARG:HD3	1:A:48:ARG:CZ	2.46	0.44
2:E:86:VAL:HG12	4:E:210:HOH:O	2.17	0.44
1:D:143:THR:CG2	3:Q:9:CYS:HB2	2.47	0.44
1:A:106:ASP:N	1:A:106:ASP:OD1	2.49	0.44
1:D:143:THR:HG21	3:Q:9:CYS:HB2	2.00	0.44
1:D:130:LEU:HD11	4:D:359:HOH:O	2.17	0.43
1:D:187:THR:HA	1:D:204:TRP:O	2.17	0.43
1:D:34:VAL:CG1	1:D:45:MET:CE	2.95	0.43
1:D:11:SER:OG	1:D:22:PHE:HD1	2.01	0.43
1:D:143:THR:HG23	3:Q:9:CYS:HA	1.99	0.43
1:A:19:GLU:HB3	1:A:20:PRO:CD	2.48	0.43
1:D:9:PHE:CD2	1:D:97:ARG:HG2	2.54	0.43
1:D:97:ARG:CZ	1:D:116:TYR:HE1	2.32	0.42
1:D:266:LEU:HA	1:D:267:PRO:HD2	1.88	0.42
3:Q:3:THR:OG1	3:Q:4:GLU:N	2.52	0.42
1:D:34:VAL:CG1	1:D:45:MET:HE2	2.49	0.42
1:D:155:GLN:NE2	4:D:310:HOH:O	2.53	0.41
1:D:35:ARG:HH11	1:D:48:ARG:NH2	2.16	0.41
1:A:35:ARG:HG3	1:A:35:ARG:O	2.20	0.41
1:D:202:ARG:CD	1:D:244:TRP:CD2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:VAL:HA	2:B:82:ARG:O	2.21	0.41
1:D:47:PRO:HB3	1:D:52:ILE:HG23	2.02	0.41
2:E:26:CYS:HB2	2:E:40:LEU:HD21	2.02	0.41
1:D:67:VAL:HB	3:Q:2:MET:HE1	2.02	0.40
1:D:131:ARG:HH11	1:D:131:ARG:HG2	1.86	0.40
2:B:7:LYS:HB2	2:B:7:LYS:HE3	1.87	0.40
2:E:42:LYS:O	2:E:43:ASN:C	2.60	0.40

All (2) 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:D:383:HOH:O	4:P:103:HOH:O[1_556]	1.56	0.64
4:A:441:HOH:O	4:D:373:HOH:O[1_554]	1.99	0.21

## 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	273/293 (93%)	264 (97%)	9 (3%)	0	100	100
1	D	273/293 (93%)	262 (96%)	9 (3%)	2 (1%)	22	30
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	E	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	P	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	Q	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	756/804 (94%)	729 (96%)	25 (3%)	2 (0%)	41	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	54	GLN
1	D	267	PRO

### 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	225/245 (92%)	218 (97%)	7 (3%)	40	57
1	D	218/245 (89%)	212 (97%)	6 (3%)	43	61
2	B	86/95 (90%)	85 (99%)	1 (1%)	71	84
2	E	87/95 (92%)	84 (97%)	3 (3%)	37	53
3	P	9/9 (100%)	7 (78%)	2 (22%)	1	1
3	Q	9/9 (100%)	9 (100%)	0	100	100
All	All	634/698 (91%)	615 (97%)	19 (3%)	41	59

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	MET
1	A	67	VAL
1	A	72	GLN
1	A	81	LEU
1	A	82	ARG
1	A	105	SER
1	A	207	SER
2	B	95	LYS
1	D	34	VAL
1	D	48	ARG
1	D	89	GLU
1	D	113	TYR
1	D	121	LYS
1	D	222	GLU
2	E	1	MET
2	E	71	PHE
2	E	78	GLU

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Mol	Chain	Res	Type
3	P	6	VAL
3	P	8	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	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 monosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	275/293 (93%)	-0.02	5 (1%) 68 70	19, 34, 56, 85	0
1	D	275/293 (93%)	0.22	14 (5%) 28 30	21, 43, 64, 165	0
2	B	100/100 (100%)	0.25	3 (3%) 50 53	22, 44, 69, 103	0
2	E	100/100 (100%)	-0.13	0 100 100	21, 38, 60, 68	0
3	P	9/9 (100%)	0.18	0 100 100	11, 25, 30, 31	0
3	Q	9/9 (100%)	0.52	0 100 100	40, 55, 63, 74	0
All	All	768/804 (95%)	0.10	22 (2%) 51 53	11, 39, 65, 165	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	96	GLN	8.9
1	A	194	VAL	5.9
1	A	16	GLY	3.2
1	D	88	SER	3.2
1	D	145	HIS	3.1
1	D	24	ALA	3.0
1	D	11	SER	2.7
1	D	130	LEU	2.7
2	B	74	THR	2.7
1	A	90	ALA	2.5
1	D	97	ARG	2.5
1	D	25	VAL	2.4
1	D	116	TYR	2.4
1	A	15	PRO	2.4
1	D	138	MET	2.4
1	D	141	GLN	2.3
1	D	40	ALA	2.2
1	D	107	TRP	2.1
2	B	79	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	98	MET	2.0
1	A	193	ALA	2.0
2	B	98	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.