



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 02:19 pm BST

PDB ID : 3BZF  
Title : The human non-classical major histocompatibility complex molecule HLA-E  
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Deposited on : 2008-01-17  
Resolution : 2.50 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	:	2.11
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)	:	2.11

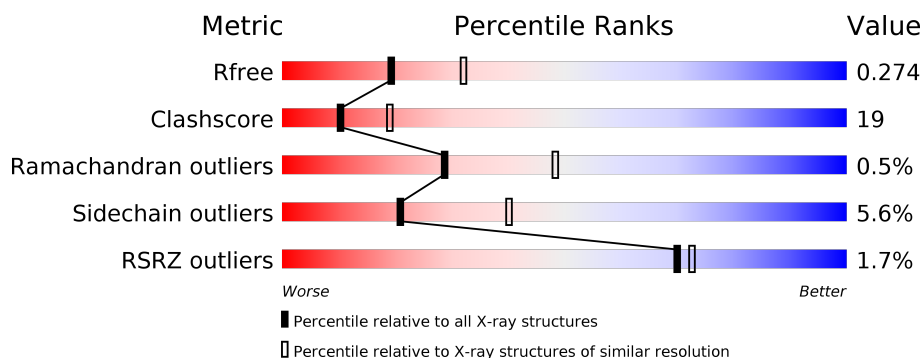
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	276	<div> <div>2%</div> <div>58% 34% 6% •</div> </div>
1	C	276	<div> <div>2%</div> <div>61% 29% 8% •</div> </div>
2	B	97	<div> <div>2%</div> <div>56% 37% 7%</div> </div>
2	D	97	<div> <div>56% 36% 8%</div> </div>
3	P	9	<div> <div>56% 44%</div> </div>
3	Q	9	<div> <div>78% 22%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6516 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, alpha chain E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2253	1409	405	432	7			
1	C	276	Total	C	N	O	S	0	0	0
			2253	1409	405	432	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			812	517	137	155	3			
2	D	97	Total	C	N	O	S	0	0	0
			812	517	137	155	3			

- Molecule 3 is a protein called leader peptide of HLA class I histocompatibility antigen, Cw-7 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	S	0	0	0
			68	45	12	10	1			
3	Q	9	Total	C	N	O	S	0	0	0
			68	45	12	10	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total	O	0	0
			82	82		
4	B	42	Total	O	0	0
			42	42		
4	P	2	Total	O	0	0
			2	2		
4	C	85	Total	O	0	0
			85	85		

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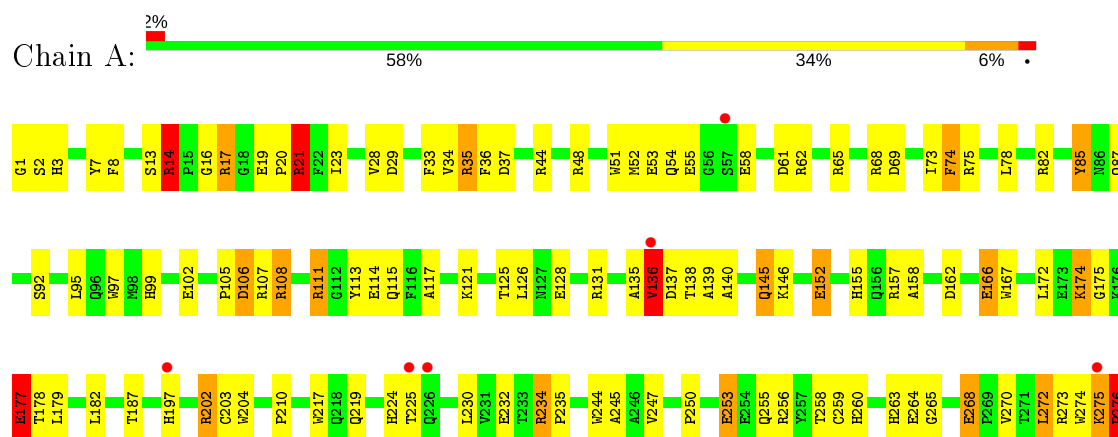
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	36	Total	O	0	0
			36	36		
4	Q	3	Total	O	0	0
			3	3		

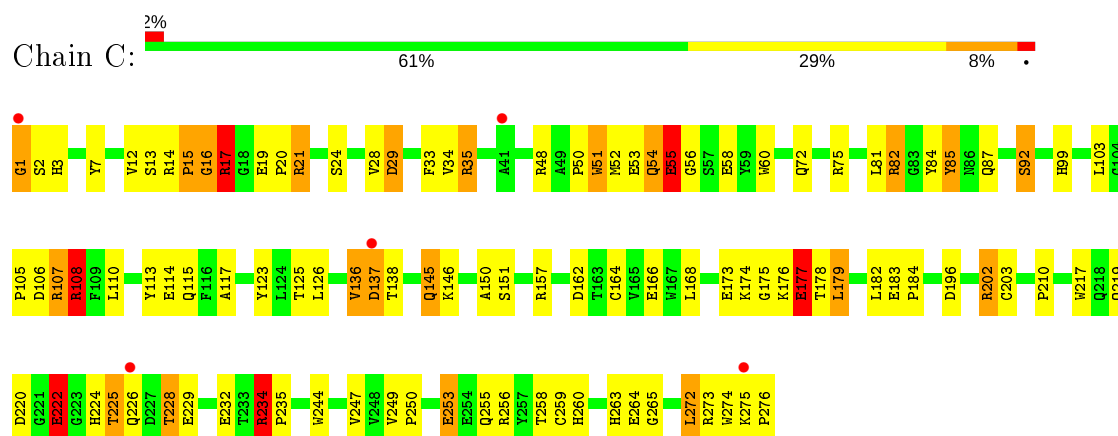
### 3 Residue-property plots [i](#)

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.

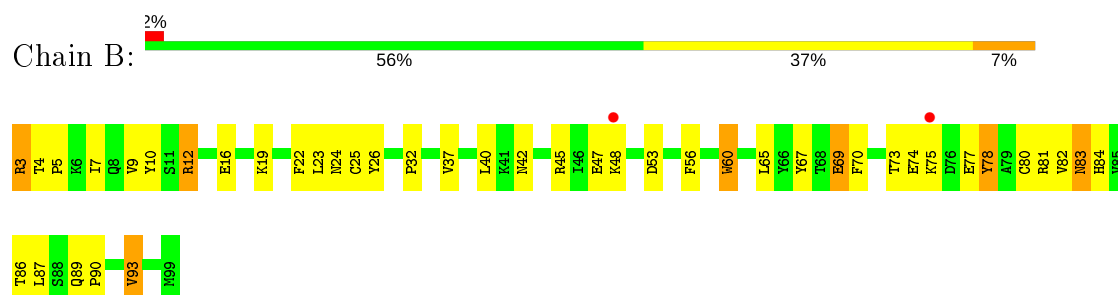
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



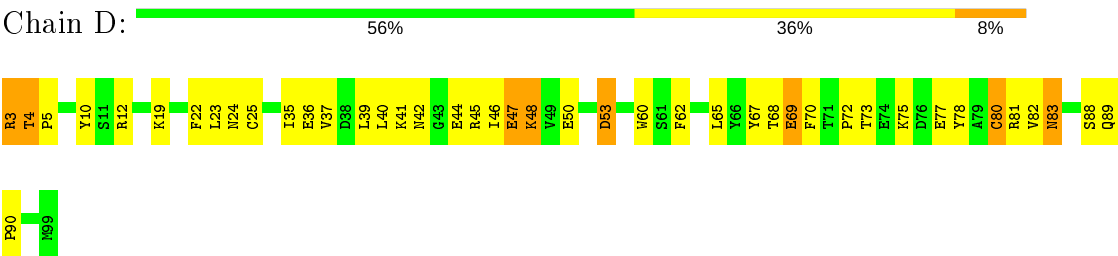
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



- Molecule 2: Beta-2-microglobulin



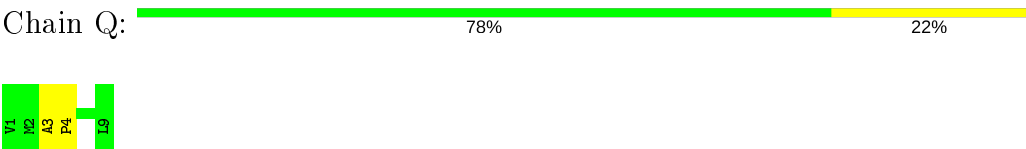
● Molecule 2: Beta-2-microglobulin



● Molecule 3: leader peptide of HLA class I histocompatibility antigen, Cw-7 alpha chain



● Molecule 3: leader peptide of HLA class I histocompatibility antigen, Cw-7 alpha chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.52Å 62.30Å 98.77Å 90.00° 106.15° 90.00°	Depositor
Resolution (Å)	29.60 – 2.50 29.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.60-2.50) 98.7 (29.60-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.200 , 0.269 0.208 , 0.274	Depositor DCC
$R_{free}$ test set	1620 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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	1.73	29/2320 (1.2%)	1.25	18/3155 (0.6%)
1	C	1.70	29/2320 (1.2%)	1.33	20/3155 (0.6%)
2	B	1.66	6/835 (0.7%)	1.18	3/1129 (0.3%)
2	D	1.64	8/835 (1.0%)	1.24	4/1129 (0.4%)
3	P	1.50	0/68	1.28	0/90
3	Q	1.46	0/68	1.24	0/90
All	All	1.69	72/6446 (1.1%)	1.27	45/8748 (0.5%)

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	A	0	2
1	C	0	2
All	All	0	4

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	GLU	CB-CG	12.64	1.76	1.52
1	C	177	GLU	CD-OE1	10.84	1.37	1.25
1	C	166	GLU	CG-CD	10.63	1.67	1.51
1	C	58	GLU	CD-OE1	10.37	1.37	1.25
1	A	177	GLU	CG-CD	10.06	1.67	1.51
1	A	232	GLU	CD-OE1	9.79	1.36	1.25
1	A	136	VAL	CB-CG1	9.50	1.72	1.52
1	C	58	GLU	CG-CD	9.36	1.66	1.51
1	C	166	GLU	CB-CG	9.02	1.69	1.52
1	A	166	GLU	CG-CD	8.83	1.65	1.51
1	A	247	VAL	CB-CG2	-8.45	1.35	1.52
1	C	232	GLU	CD-OE1	7.95	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	ARG	CZ-NH1	-7.89	1.22	1.33
2	B	26	TYR	CD1-CE1	7.71	1.50	1.39
2	B	80	CYS	CB-SG	7.65	1.95	1.82
1	C	19	GLU	CD-OE2	7.65	1.34	1.25
1	C	229	GLU	CD-OE2	-7.53	1.17	1.25
1	A	58	GLU	CD-OE1	7.36	1.33	1.25
2	B	60	TRP	CG-CD1	-7.16	1.26	1.36
1	C	145	GLN	CG-CD	7.05	1.67	1.51
1	A	268	GLU	CG-CD	6.85	1.62	1.51
2	D	69	GLU	CG-CD	6.81	1.62	1.51
2	D	80	CYS	CB-SG	6.74	1.93	1.82
1	A	253	GLU	CD-OE1	6.71	1.33	1.25
1	A	167	TRP	CG-CD1	-6.62	1.27	1.36
1	A	152	GLU	CB-CG	6.60	1.64	1.52
1	C	85	TYR	CG-CD2	-6.57	1.30	1.39
2	D	44	GLU	CB-CG	6.55	1.64	1.52
1	A	58	GLU	CG-CD	6.44	1.61	1.51
1	C	1	GLY	N-CA	6.37	1.55	1.46
1	C	84	TYR	CD2-CE2	-6.09	1.30	1.39
1	C	113	TYR	CE1-CZ	6.08	1.46	1.38
2	D	44	GLU	CD-OE1	6.08	1.32	1.25
1	C	123	TYR	CD2-CE2	6.06	1.48	1.39
2	B	78	TYR	CB-CG	6.03	1.60	1.51
1	A	145	GLN	CG-CD	6.00	1.64	1.51
1	A	65	ARG	CZ-NH2	-5.99	1.25	1.33
2	B	69	GLU	CG-CD	5.97	1.60	1.51
2	D	62	PHE	CE2-CZ	5.96	1.48	1.37
1	C	164	CYS	CB-SG	5.94	1.92	1.82
1	A	276	PRO	C-O	5.88	1.35	1.23
1	A	113	TYR	CE2-CZ	5.81	1.46	1.38
1	C	107	ARG	CG-CD	5.72	1.66	1.51
1	C	56	GLY	CA-C	-5.72	1.42	1.51
1	C	51	TRP	CB-CG	-5.61	1.40	1.50
1	A	128	GLU	CG-CD	5.56	1.60	1.51
1	A	139	ALA	CA-CB	5.47	1.64	1.52
2	D	35	ILE	N-CA	-5.43	1.35	1.46
2	D	48	LYS	CB-CG	5.39	1.67	1.52
1	C	12	VAL	CB-CG1	-5.39	1.41	1.52
1	A	44	ARG	CZ-NH1	-5.37	1.26	1.33
2	B	26	TYR	CD2-CE2	5.36	1.47	1.39
1	C	253	GLU	CD-OE1	5.29	1.31	1.25
1	C	173	GLU	CD-OE1	5.26	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	17	ARG	NE-CZ	5.25	1.39	1.33
1	A	74	PHE	CE1-CZ	-5.24	1.27	1.37
1	A	275	LYS	C-O	5.22	1.33	1.23
1	A	166	GLU	CD-OE1	5.20	1.31	1.25
2	D	48	LYS	C-O	5.18	1.33	1.23
1	C	177	GLU	CG-CD	5.18	1.59	1.51
1	A	174	LYS	CD-CE	5.17	1.64	1.51
1	C	72	GLN	CD-NE2	5.16	1.45	1.32
1	A	128	GLU	CB-CG	5.16	1.61	1.52
1	C	54	GLN	CB-CG	5.16	1.66	1.52
1	A	247	VAL	C-O	-5.10	1.13	1.23
1	A	97	TRP	CE2-CZ2	5.08	1.48	1.39
1	C	24	SER	CB-OG	5.07	1.48	1.42
1	C	123	TYR	CD1-CE1	5.05	1.47	1.39
1	C	16	GLY	C-O	-5.04	1.15	1.23
1	A	19	GLU	CG-CD	5.04	1.59	1.51
1	A	85	TYR	C-O	5.04	1.32	1.23
1	C	60	TRP	CB-CG	-5.00	1.41	1.50

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	ARG	NE-CZ-NH2	-17.19	111.70	120.30
1	C	202	ARG	NE-CZ-NH1	11.93	126.27	120.30
1	C	82	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	C	202	ARG	CD-NE-CZ	9.08	136.31	123.60
1	A	276	PRO	N-CA-C	9.01	135.51	112.10
2	B	12	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	C	55	GLU	N-CA-C	-8.38	88.39	111.00
1	A	37	ASP	CB-CG-OD2	-8.16	110.96	118.30
1	A	202	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	21	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	C	234	ARG	NE-CZ-NH1	7.48	124.04	120.30
2	D	47	GLU	C-N-CA	-7.30	103.46	121.70
2	D	53	ASP	CB-CG-OD1	7.03	124.62	118.30
1	A	61	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	75	ARG	NE-CZ-NH1	6.64	123.62	120.30
2	D	81	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	37	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	111	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	A	106	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	A	62	ARG	NE-CZ-NH1	6.28	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	PRO	CB-CA-C	-6.21	96.48	112.00
1	A	131	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	C	196	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	C	234	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	162	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	137	ASP	CB-CG-OD1	-5.95	112.95	118.30
1	C	15	PRO	CB-CA-C	-5.91	97.23	112.00
1	C	108	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	14	ARG	N-CA-C	-5.80	95.34	111.00
1	C	247	VAL	CG1-CB-CG2	5.80	120.18	110.90
2	D	3	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	272	LEU	CB-CG-CD2	-5.71	101.28	111.00
2	B	25	CYS	CA-CB-SG	-5.70	103.74	114.00
2	B	87	LEU	CB-CG-CD1	-5.69	101.32	111.00
1	C	54	GLN	N-CA-C	-5.67	95.69	111.00
1	C	75	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	C	14	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	C	166	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	A	69	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	222	GLU	O-C-N	-5.35	114.11	123.20
1	C	17	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	108	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	137	ASP	CB-CA-C	5.17	120.74	110.40
1	C	272	LEU	CA-CB-CG	5.07	126.96	115.30
1	C	222	GLU	CA-C-O	5.04	130.68	120.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ARG	Mainchain
1	A	275	LYS	Mainchain
1	C	222	GLU	Mainchain
1	C	275	LYS	Mainchain

## 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	2253	0	2098	83	0
1	C	2253	0	2098	79	0
2	B	812	0	772	40	0
2	D	812	0	774	36	0
3	P	68	0	83	5	0
3	Q	68	0	83	2	0
4	A	82	0	0	5	0
4	B	42	0	0	4	0
4	C	85	0	0	9	0
4	D	36	0	0	2	0
4	P	2	0	0	2	0
4	Q	3	0	0	2	0
All	All	6516	0	5908	227	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 19.

All (227) 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:A:177:GLU:CB	1:A:177:GLU:CG	1.76	1.61
1:C:228:THR:CG2	4:C:415:HOH:O	1.97	1.13
1:C:15:PRO:O	1:C:17:ARG:NH1	1.82	1.11
2:D:47:GLU:HB2	2:D:48:LYS:HD3	1.35	1.08
1:A:121:LYS:HD2	4:A:339:HOH:O	1.53	1.06
1:C:48:ARG:NH1	2:D:53:ASP:OD2	1.87	1.06
2:D:47:GLU:O	2:D:48:LYS:HB2	1.49	1.06
1:C:228:THR:HG21	4:C:415:HOH:O	1.58	1.00
1:A:16:GLY:H	1:A:17:ARG:NH1	1.59	1.00
1:C:21:ARG:HD3	4:C:378:HOH:O	1.60	0.99
2:D:47:GLU:HB2	2:D:48:LYS:CD	1.92	0.97
1:A:16:GLY:H	1:A:17:ARG:HH11	0.98	0.92
1:C:54:GLN:O	1:C:55:GLU:HB2	1.74	0.88
2:D:47:GLU:O	2:D:48:LYS:CB	2.14	0.85
1:A:21:ARG:NE	1:A:23:ILE:HD11	1.90	0.84
1:A:121:LYS:HE2	4:A:317:HOH:O	1.78	0.82
2:D:83:ASN:ND2	2:D:90:PRO:HB3	1.95	0.81
2:B:73:THR:HG22	2:B:74:GLU:N	1.96	0.81
1:A:82:ARG:O	1:A:85:TYR:O	2.00	0.80
1:C:250:PRO:HB2	1:C:253:GLU:HG3	1.64	0.78
1:A:108:ARG:HH11	1:A:108:ARG:HB2	1.50	0.77
1:C:136:VAL:O	1:C:137:ASP:CG	2.24	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:THR:HG22	2:B:74:GLU:H	1.49	0.76
1:C:202:ARG:HD2	1:C:244:TRP:CD2	2.20	0.75
1:C:222:GLU:OE2	4:C:414:HOH:O	2.05	0.75
1:A:21:ARG:HE	1:A:23:ILE:HD11	1.49	0.74
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.23	0.73
1:C:35:ARG:NH1	2:D:53:ASP:OD1	2.21	0.72
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.25	0.72
1:A:16:GLY:N	1:A:17:ARG:HH11	1.81	0.72
1:A:263:HIS:CD2	1:A:265:GLY:H	2.08	0.71
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.26	0.70
1:C:234:ARG:HD3	2:D:10:TYR:CZ	2.26	0.70
1:C:225:THR:C	1:C:228:THR:OG1	2.30	0.70
1:A:108:ARG:HB2	1:A:108:ARG:NH1	2.07	0.69
1:C:263:HIS:CD2	1:C:265:GLY:H	2.10	0.69
1:A:48:ARG:NH1	2:B:53:ASP:OD2	2.26	0.68
1:C:106:ASP:OD1	1:C:108:ARG:HG3	1.92	0.68
1:A:13:SER:HA	1:A:20:PRO:HB3	1.77	0.67
1:C:13:SER:HA	1:C:20:PRO:HB3	1.75	0.67
1:A:250:PRO:HB2	1:A:253:GLU:HG3	1.75	0.67
3:P:6:ALA:O	4:P:115:HOH:O	2.12	0.67
1:C:225:THR:O	1:C:228:THR:OG1	2.13	0.65
1:A:106:ASP:O	1:A:107:ARG:HB2	1.95	0.65
1:A:255:GLN:OE1	1:A:273:ARG:HD3	1.97	0.65
1:A:16:GLY:N	1:A:17:ARG:NH1	2.39	0.65
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.32	0.64
1:C:175:GLY:O	1:C:179:LEU:HB2	1.97	0.64
1:A:13:SER:O	1:A:92:SER:HB2	1.98	0.62
3:Q:3:ALA:HB1	4:Q:12:HOH:O	1.98	0.62
1:C:157:ARG:HD3	4:C:357:HOH:O	2.00	0.62
2:B:73:THR:HG21	2:B:75:LYS:NZ	2.15	0.62
1:C:125:THR:HG22	1:C:126:LEU:O	2.00	0.62
1:C:1:GLY:N	1:C:107:ARG:HE	1.97	0.61
1:C:54:GLN:O	1:C:54:GLN:CD	2.39	0.61
1:C:82:ARG:O	1:C:85:TYR:O	2.17	0.61
1:A:125:THR:HG22	1:A:126:LEU:O	2.01	0.61
1:A:155:HIS:HE1	4:A:326:HOH:O	1.84	0.60
2:D:47:GLU:O	2:D:48:LYS:C	2.36	0.60
2:D:46:ILE:HG22	2:D:47:GLU:O	2.02	0.60
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.84	0.60
2:D:24:ASN:HB3	2:D:65:LEU:HD11	1.84	0.59
1:A:157:ARG:HD3	4:A:321:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.84	0.59
2:D:47:GLU:HB2	2:D:48:LYS:CG	2.32	0.59
2:D:40:LEU:HD23	2:D:45:ARG:HA	1.84	0.59
1:C:13:SER:O	1:C:92:SER:HB2	2.02	0.59
2:D:25:CYS:CB	2:D:80:CYS:SG	2.91	0.59
1:C:234:ARG:HD3	2:D:10:TYR:CE1	2.38	0.58
1:A:108:ARG:HH11	1:A:108:ARG:CB	2.15	0.58
1:A:162:ASP:C	1:A:166:GLU:OE1	2.42	0.58
1:C:50:PRO:O	1:C:53:GLU:HB2	2.04	0.58
1:A:1:GLY:N	1:A:107:ARG:HE	2.02	0.58
1:C:182:LEU:HD13	1:C:264:GLU:HG2	1.86	0.57
1:C:15:PRO:C	1:C:17:ARG:NH1	2.57	0.57
1:C:28:VAL:O	1:C:29:ASP:HB2	2.05	0.57
2:D:42:ASN:ND2	2:D:77:GLU:H	2.03	0.57
2:B:9:VAL:CG2	2:B:93:VAL:HG22	2.35	0.56
1:A:175:GLY:O	1:A:179:LEU:HB2	2.04	0.56
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.40	0.56
1:C:99:HIS:HB3	1:C:114:GLU:HG3	1.88	0.56
2:D:22:PHE:CE1	2:D:69:GLU:HG2	2.41	0.56
2:B:73:THR:CG2	2:B:74:GLU:N	2.67	0.56
1:A:253:GLU:O	1:A:256:ARG:HB2	2.06	0.55
1:C:106:ASP:OD2	1:C:108:ARG:NH1	2.39	0.55
1:A:99:HIS:HB3	1:A:114:GLU:HG3	1.88	0.55
1:C:52:MET:HE3	1:C:174:LYS:HD2	1.89	0.55
2:D:19:LYS:O	2:D:72:PRO:HD2	2.06	0.55
2:B:42:ASN:ND2	2:B:77:GLU:H	2.05	0.55
1:C:234:ARG:HD3	2:D:10:TYR:CE2	2.41	0.55
1:A:225:THR:HG22	1:A:225:THR:O	2.07	0.55
1:A:82:ARG:HG2	1:A:87:GLN:HB2	1.89	0.55
1:C:54:GLN:O	1:C:54:GLN:CG	2.53	0.54
2:B:3:ARG:HB2	2:B:3:ARG:HH11	1.73	0.54
1:A:17:ARG:HD3	1:A:17:ARG:N	2.22	0.54
2:D:41:LYS:O	2:D:42:ASN:HB2	2.07	0.54
3:P:4:PRO:HD2	4:P:41:HOH:O	2.08	0.54
1:A:177:GLU:CG	1:A:177:GLU:CA	2.77	0.54
1:C:203:CYS:HB2	1:C:217:TRP:CZ2	2.43	0.53
2:D:42:ASN:HD21	2:D:77:GLU:H	1.55	0.53
1:A:182:LEU:HD13	1:A:264:GLU:HG2	1.91	0.53
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.44	0.53
1:C:82:ARG:HG2	1:C:87:GLN:HB2	1.90	0.53
1:A:102:GLU:OE2	1:A:111:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLN:HG2	1:A:224:HIS:CD2	2.45	0.52
1:C:225:THR:C	1:C:228:THR:HG1	2.05	0.52
1:C:274:TRP:CH2	1:C:276:PRO:HB3	2.44	0.52
1:A:219:GLN:O	1:A:219:GLN:HG3	2.09	0.52
3:Q:4:PRO:HD2	4:Q:12:HOH:O	2.08	0.52
1:C:210:PRO:O	1:C:263:HIS:HE1	1.92	0.52
1:C:226:GLN:HG2	4:C:423:HOH:O	2.08	0.52
1:A:162:ASP:HB3	1:A:166:GLU:OE1	2.10	0.51
2:B:73:THR:CG2	2:B:74:GLU:H	2.21	0.51
2:B:81:ARG:HD2	4:B:127:HOH:O	2.09	0.51
1:C:17:ARG:HD3	1:C:17:ARG:N	2.25	0.51
1:C:106:ASP:O	1:C:107:ARG:HB2	2.11	0.51
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.47	0.50
2:B:73:THR:HG21	2:B:75:LYS:HZ1	1.75	0.50
2:B:83:ASN:ND2	2:B:90:PRO:HB3	2.27	0.50
1:A:21:ARG:HE	1:A:23:ILE:CD1	2.19	0.49
1:C:103:LEU:HG	1:C:168:LEU:HD23	1.93	0.49
1:A:121:LYS:CE	4:A:317:HOH:O	2.48	0.49
1:C:258:THR:OG1	1:C:260:HIS:HE1	1.96	0.49
2:B:23:LEU:O	2:B:67:TYR:HA	2.13	0.49
1:C:219:GLN:HG2	1:C:224:HIS:CD2	2.48	0.48
1:C:7:TYR:HB2	1:C:99:HIS:CE1	2.48	0.48
2:D:39:LEU:HD23	2:D:68:THR:HG22	1.96	0.48
2:B:42:ASN:HD21	2:B:77:GLU:H	1.61	0.48
2:D:41:LYS:HB3	4:D:109:HOH:O	2.13	0.48
1:A:106:ASP:O	1:A:107:ARG:CB	2.62	0.47
2:D:37:VAL:HG22	2:D:82:VAL:HG22	1.96	0.47
1:C:150:ALA:O	1:C:151:SER:HB3	2.15	0.47
2:B:9:VAL:HG23	2:B:93:VAL:HG22	1.97	0.47
2:B:40:LEU:O	2:B:78:TYR:HA	2.15	0.47
1:C:219:GLN:O	1:C:219:GLN:HG3	2.15	0.47
1:C:253:GLU:O	1:C:256:ARG:HB2	2.14	0.47
1:A:177:GLU:CD	1:A:178:THR:HG23	2.36	0.47
2:B:32:PRO:HB2	4:B:110:HOH:O	2.14	0.47
2:B:22:PHE:CZ	2:B:69:GLU:HG2	2.50	0.47
1:A:230:LEU:HD12	1:A:245:ALA:HB2	1.97	0.46
1:C:202:ARG:CD	1:C:244:TRP:CE3	2.98	0.46
1:A:210:PRO:O	1:A:263:HIS:HE1	1.98	0.46
2:D:73:THR:HG22	2:D:75:LYS:HG2	1.96	0.46
2:D:83:ASN:HD21	2:D:90:PRO:HB3	1.75	0.46
1:A:145:GLN:NE2	1:A:146:LYS:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:HG12	1:A:272:LEU:CD2	2.45	0.46
1:A:258:THR:OG1	1:A:260:HIS:HE1	1.99	0.46
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.97	0.46
2:D:4:THR:HG23	2:D:5:PRO:HD2	1.98	0.46
2:B:45:ARG:NH1	2:B:47:GLU:OE2	2.48	0.45
1:C:35:ARG:C	1:C:35:ARG:HD2	2.36	0.45
1:A:54:GLN:NE2	1:A:55:GLU:OE1	2.45	0.45
2:B:7:ILE:HD11	2:B:82:VAL:HB	1.99	0.45
2:B:9:VAL:HG21	2:B:93:VAL:HG22	1.98	0.45
2:B:4:THR:HG23	2:B:5:PRO:HD2	1.97	0.45
2:B:22:PHE:CE1	2:B:69:GLU:HG2	2.51	0.45
1:C:2:SER:O	1:C:3:HIS:CG	2.70	0.45
3:P:3:ALA:HA	3:P:4:PRO:HD3	1.80	0.45
1:C:1:GLY:N	4:C:397:HOH:O	2.50	0.44
1:A:274:TRP:O	1:A:276:PRO:HD3	2.16	0.44
2:D:41:LYS:HG3	2:D:78:TYR:CE1	2.52	0.44
1:A:1:GLY:HA2	1:A:105:PRO:HA	1.99	0.44
2:D:89:GLN:HB2	2:D:90:PRO:HD2	1.99	0.44
1:A:125:THR:OG1	1:A:136:VAL:HG21	2.17	0.44
1:A:52:MET:HE3	1:A:174:LYS:HD2	1.99	0.44
1:C:255:GLN:OE1	1:C:273:ARG:HD3	2.17	0.44
1:A:172:LEU:HD23	1:A:179:LEU:HD23	2.00	0.44
1:A:234:ARG:HD3	2:B:10:TYR:CE1	2.53	0.44
1:C:202:ARG:HD2	1:C:244:TRP:CE3	2.51	0.44
2:D:45:ARG:NH1	2:D:47:GLU:OE1	2.51	0.44
1:C:263:HIS:HD2	1:C:265:GLY:H	1.61	0.43
1:C:35:ARG:HG2	1:C:48:ARG:HD3	2.00	0.43
2:B:3:ARG:NH1	2:B:3:ARG:HB2	2.34	0.43
1:A:187:THR:HA	1:A:204:TRP:O	2.18	0.43
1:A:74:PHE:CD2	1:A:95:LEU:HD23	2.53	0.43
1:C:1:GLY:CA	4:C:397:HOH:O	2.66	0.43
1:C:259:CYS:HB3	1:C:272:LEU:HB2	2.00	0.43
2:D:23:LEU:O	2:D:67:TYR:HA	2.18	0.43
1:C:136:VAL:O	1:C:137:ASP:OD1	2.37	0.43
2:D:41:LYS:O	2:D:42:ASN:C	2.52	0.43
1:A:2:SER:O	1:A:3:HIS:CG	2.71	0.43
2:B:84:HIS:CE1	2:B:86:THR:HG23	2.53	0.43
1:A:35:ARG:HG2	1:A:48:ARG:HD3	2.00	0.43
2:B:3:ARG:HD2	4:B:111:HOH:O	2.18	0.43
1:C:177:GLU:OE1	1:C:178:THR:HG23	2.19	0.43
1:A:172:LEU:HA	1:A:179:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:CYS:HB3	1:A:272:LEU:HB2	2.02	0.42
1:A:158:ALA:O	1:A:162:ASP:HB2	2.19	0.42
1:A:202:ARG:HD2	1:A:244:TRP:CE3	2.52	0.42
1:C:125:THR:OG1	1:C:136:VAL:HG21	2.19	0.42
1:A:82:ARG:HA	1:A:87:GLN:HE21	1.84	0.42
2:B:16:GLU:OE2	2:B:19:LYS:HG3	2.20	0.42
1:A:16:GLY:C	1:A:17:ARG:HD3	2.39	0.42
1:C:33:PHE:CD2	1:C:34:VAL:HG13	2.54	0.42
1:A:152:GLU:HB3	3:P:7:LEU:HD21	2.02	0.42
1:A:1:GLY:H1	1:A:107:ARG:HE	1.67	0.42
1:C:51:TRP:CE3	1:C:52:MET:HG2	2.54	0.41
1:A:36:PHE:C	1:A:36:PHE:CD1	2.93	0.41
1:C:235:PRO:HG2	2:D:65:LEU:HD22	2.01	0.41
2:B:48:LYS:C	4:B:132:HOH:O	2.57	0.41
1:C:105:PRO:C	1:C:107:ARG:H	2.23	0.41
1:C:1:GLY:HA2	1:C:105:PRO:HA	2.01	0.41
1:C:176:LYS:HG3	1:C:177:GLU:H	1.86	0.41
1:C:202:ARG:HD3	1:C:244:TRP:CE3	2.55	0.41
1:C:249:VAL:HA	1:C:250:PRO:HD3	1.82	0.41
1:A:51:TRP:CE3	1:A:52:MET:HG2	2.56	0.41
1:C:81:LEU:O	1:C:85:TYR:HD1	2.03	0.41
1:C:16:GLY:C	1:C:17:ARG:HD3	2.39	0.41
2:D:88:SER:OG	2:D:89:GLN:HG2	2.20	0.41
1:C:145:GLN:NE2	1:C:146:LYS:HB2	2.35	0.41
1:A:234:ARG:HD3	2:B:10:TYR:CD2	2.56	0.41
1:A:7:TYR:HB2	1:A:99:HIS:CE1	2.55	0.41
1:C:105:PRO:C	1:C:107:ARG:N	2.75	0.41
1:C:220:ASP:OD2	1:C:256:ARG:HG2	2.21	0.41
1:A:135:ALA:HB1	1:A:140:ALA:HB3	2.02	0.41
1:A:28:VAL:O	1:A:29:ASP:HB2	2.20	0.41
1:A:13:SER:HB3	1:A:78:LEU:HD13	2.03	0.40
1:A:8:PHE:HD2	2:B:56:PHE:CE1	2.38	0.40
1:C:228:THR:HG22	4:C:415:HOH:O	1.92	0.40
2:D:50:GLU:HG2	4:D:102:HOH:O	2.22	0.40
1:A:73:ILE:HG21	3:P:6:ALA:O	2.21	0.40
1:A:230:LEU:CD1	1:A:245:ALA:HB2	2.51	0.40
2:B:73:THR:HG21	2:B:75:LYS:HZ2	1.85	0.40
2:B:73:THR:HG22	2:B:75:LYS:H	1.86	0.40
1:C:183:GLU:HA	1:C:184:PRO:HD2	1.97	0.40
1:A:234:ARG:HB2	2:B:10:TYR:OH	2.21	0.40
1:C:110:LEU:HD12	1:C:110:LEU:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/276 (99%)	259 (94%)	14 (5%)	1 (0%)	34	54
1	C	274/276 (99%)	254 (93%)	17 (6%)	3 (1%)	14	26
2	B	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
2	D	95/97 (98%)	89 (94%)	6 (6%)	0	100	100
3	P	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	Q	7/9 (78%)	7 (100%)	0	0	100	100
All	All	752/764 (98%)	706 (94%)	42 (6%)	4 (0%)	29	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	137	ASP
1	A	177	GLU
1	C	29	ASP
1	C	55	GLU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/238 (100%)	225 (94%)	13 (6%)	21	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	238/238 (100%)	225 (94%)	13 (6%)	21	41
2	B	92/92 (100%)	86 (94%)	6 (6%)	17	33
2	D	92/92 (100%)	86 (94%)	6 (6%)	17	33
3	P	7/7 (100%)	7 (100%)	0	100	100
3	Q	7/7 (100%)	7 (100%)	0	100	100
All	All	674/674 (100%)	636 (94%)	38 (6%)	21	40

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	ARG
1	A	21	ARG
1	A	35	ARG
1	A	53	GLU
1	A	115	GLN
1	A	136	VAL
1	A	138	THR
1	A	177	GLU
1	A	197	HIS
1	A	234	ARG
1	A	268	GLU
1	A	276	PRO
2	B	3	ARG
2	B	12	ARG
2	B	70	PHE
2	B	83	ASN
2	B	89	GLN
2	B	93	VAL
1	C	17	ARG
1	C	21	ARG
1	C	35	ARG
1	C	92	SER
1	C	108	ARG
1	C	115	GLN
1	C	136	VAL
1	C	138	THR
1	C	177	GLU
1	C	179	LEU
1	C	225	THR

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Mol	Chain	Res	Type
1	C	228	THR
1	C	234	ARG
2	D	3	ARG
2	D	4	THR
2	D	12	ARG
2	D	36	GLU
2	D	70	PHE
2	D	83	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	87	GLN
1	A	115	GLN
1	A	127	ASN
1	A	141	GLN
1	A	145	GLN
1	A	156	GLN
1	A	218	GLN
1	A	224	HIS
1	A	260	HIS
1	A	263	HIS
2	B	42	ASN
2	B	83	ASN
1	C	72	GLN
1	C	87	GLN
1	C	115	GLN
1	C	127	ASN
1	C	145	GLN
1	C	218	GLN
1	C	224	HIS
1	C	260	HIS
1	C	263	HIS
2	D	42	ASN
2	D	83	ASN

### 5.3.3 RNA ⓘ

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 [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	276/276 (100%)	-0.30	6 (2%) 62 65	21, 32, 50, 66	0
1	C	276/276 (100%)	-0.26	5 (1%) 68 71	23, 33, 52, 63	0
2	B	97/97 (100%)	-0.22	2 (2%) 63 66	24, 34, 51, 60	0
2	D	97/97 (100%)	-0.09	0 100 100	24, 38, 53, 64	0
3	P	9/9 (100%)	-0.04	0 100 100	21, 27, 33, 35	0
3	Q	9/9 (100%)	0.24	0 100 100	26, 29, 32, 33	0
All	All	764/764 (100%)	-0.24	13 (1%) 70 72	21, 33, 52, 66	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	137	ASP	3.7
1	A	275	LYS	3.3
1	C	41	ALA	3.1
1	C	1	GLY	2.6
1	C	275	LYS	2.4
1	A	57	SER	2.3
2	B	48	LYS	2.3
1	A	197	HIS	2.2
1	A	225	THR	2.2
1	A	136	VAL	2.1
1	C	226	GLN	2.1
2	B	75	LYS	2.0
1	A	226	GLN	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.