



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:09 PM UTC

PDB ID : 4E5X / pdb\_00004e5x  
Title : Crystal structure of a complex between the human adenovirus type 2 E3-19K protein and MHC class I molecule HLA-A2/Tax  
Authors : Li, L.; Bouvier, M.  
Deposited on : 2012-03-14  
Resolution : 1.95 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

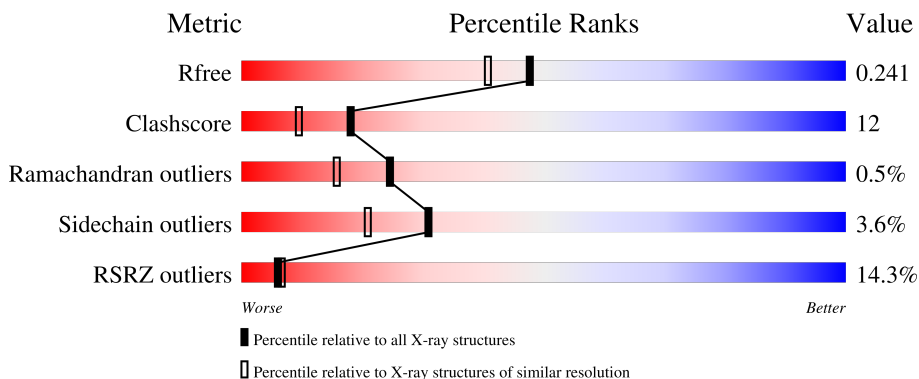
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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.



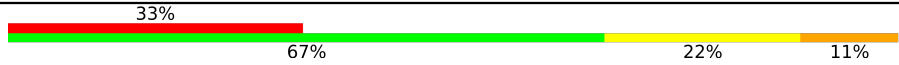

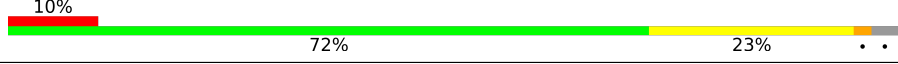
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 of 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	275	 15% 77% 20%
1	D	275	 20% 65% 31%
2	B	100	 13% 78% 21%
2	E	100	 9% 87% 13%
3	C	9	 11% 78% 22%

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Mol	Chain	Length	Quality of chain
3	F	9	
4	G	100	
4	H	100	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8439 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-2 alpha chain.

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

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

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

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 Protein Tax-1.

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

- Molecule 4 is a protein called Early E3 18.5 kDa glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	99	Total	C	N	O	S	0	0	0
			832	539	134	151	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	97	813	528	130	147	8	0	0	0

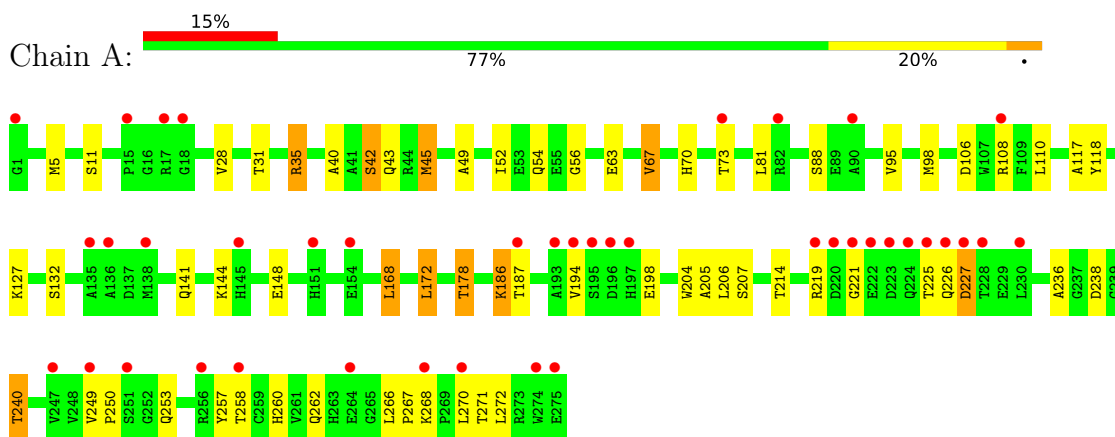
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	107	Total	O	0	0
			107	107		
5	B	52	Total	O	0	0
			52	52		
5	C	10	Total	O	0	0
			10	10		
5	D	101	Total	O	0	0
			101	101		
5	E	35	Total	O	0	0
			35	35		
5	F	4	Total	O	0	0
			4	4		
5	G	82	Total	O	0	0
			82	82		
5	H	81	Total	O	0	0
			81	81		

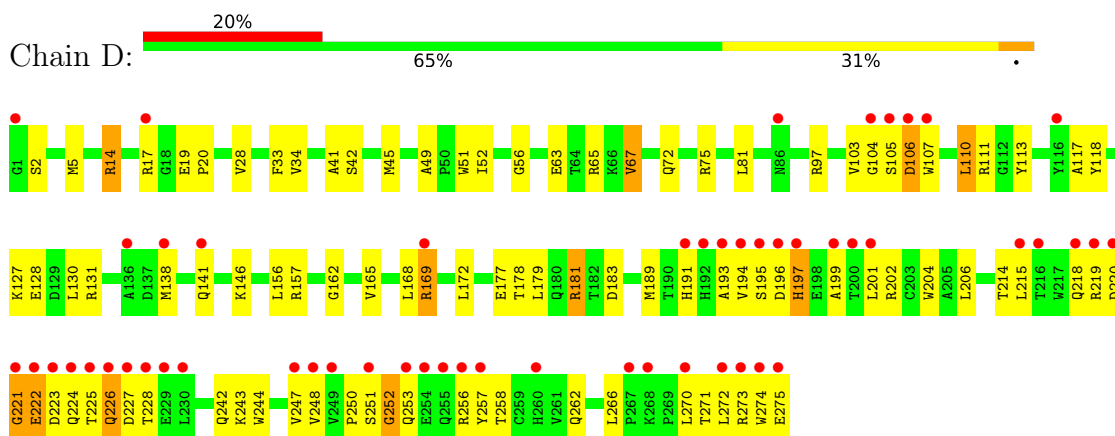
### 3 Residue-property plots [i](#)

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.

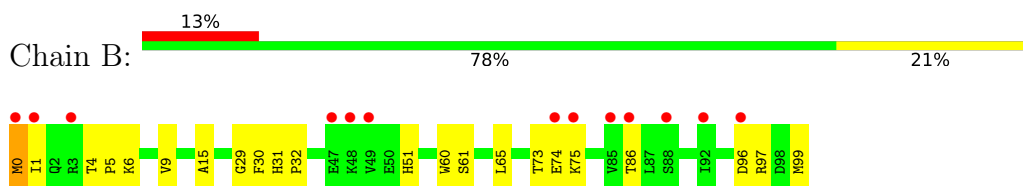
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



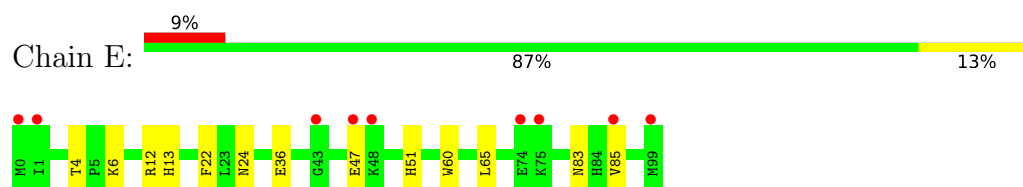
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



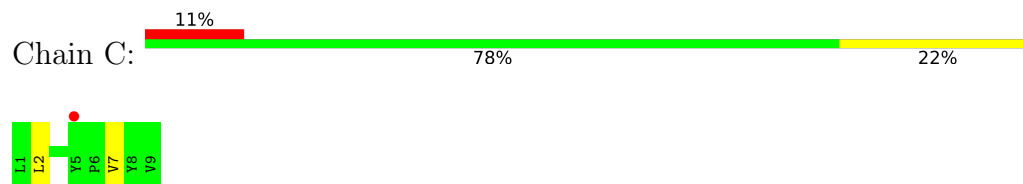
- Molecule 2: Beta-2-microglobulin



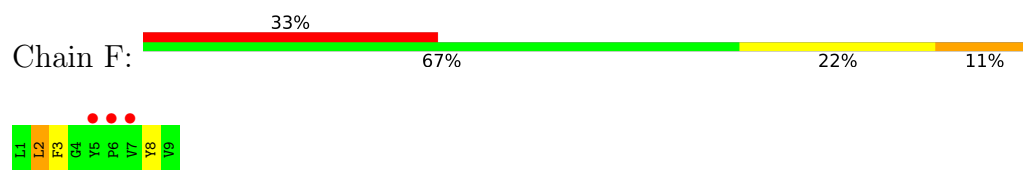
- Molecule 2: Beta-2-microglobulin



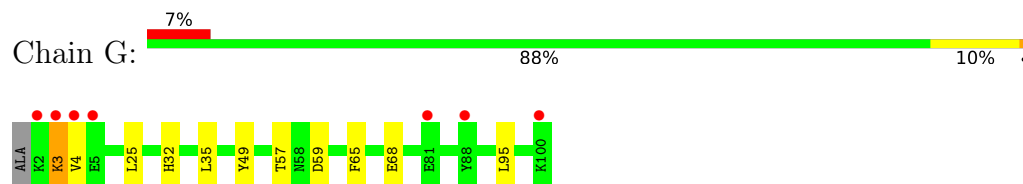
- Molecule 3: Protein Tax-1



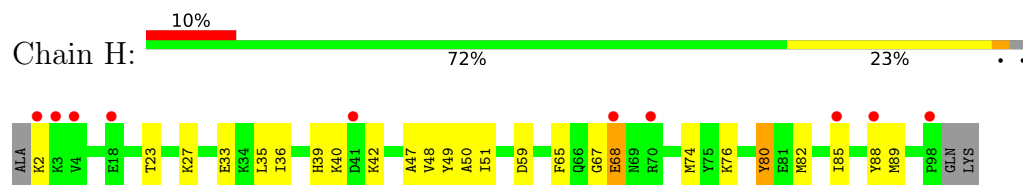
- Molecule 3: Protein Tax-1



- Molecule 4: Early E3 18.5 kDa glycoprotein



- Molecule 4: Early E3 18.5 kDa glycoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.19Å 133.67Å 196.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.06 – 1.95 37.06 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.9 (37.06-1.95) 95.0 (37.06-1.95)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 1.95Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.210 , 0.241 0.210 , 0.241	Depositor DCC
$R_{free}$ test set	10808 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtrriage
Anisotropy	0.497	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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 i

### 5.1 Standard geometry i

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	0.35	0/2312	0.86	8/3137 (0.3%)
1	D	0.36	0/2312	0.89	9/3137 (0.3%)
2	B	0.35	0/860	0.90	4/1162 (0.3%)
2	E	0.32	0/860	0.87	2/1162 (0.2%)
3	C	0.56	0/80	0.95	0/108
3	F	0.46	0/80	1.06	1/108 (0.9%)
4	G	0.40	0/855	0.79	0/1150
4	H	0.38	0/836	0.80	1/1127 (0.1%)
All	All	0.36	0/8195	0.86	25/11091 (0.2%)

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
4	H	0	1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	47	GLU	N-CA-C	9.14	121.17	111.03
2	B	0	MET	CA-C-N	-7.47	112.56	122.94
2	B	0	MET	C-N-CA	-7.47	112.56	122.94
1	A	45	MET	N-CA-C	-7.08	99.79	110.28
2	E	6	LYS	N-CA-C	-6.78	99.55	110.32
1	D	45	MET	N-CA-C	-6.57	100.11	109.96
1	A	28	VAL	N-CA-C	-6.38	98.44	107.75
1	D	56	GLY	CA-C-N	5.99	126.15	119.32
1	D	56	GLY	C-N-CA	5.99	126.15	119.32
2	B	6	LYS	N-CA-C	-5.81	101.08	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	VAL	N-CA-C	-5.77	98.11	107.28
1	D	220	ASP	N-CA-C	-5.74	103.99	111.74
1	A	42	SER	N-CA-C	5.64	117.43	111.28
2	B	15	ALA	N-CA-C	5.54	118.48	110.28
3	F	3	PHE	N-CA-C	-5.50	102.14	110.28
1	A	56	GLY	CA-C-N	5.41	125.49	119.32
1	A	56	GLY	C-N-CA	5.41	125.49	119.32
1	D	221	GLY	N-CA-C	-5.41	101.09	112.45
1	A	227	ASP	N-CA-C	-5.32	106.80	113.72
1	D	106	ASP	N-CA-C	-5.32	100.09	109.02
1	A	186	LYS	N-CA-C	-5.26	100.16	108.73
1	A	54	GLN	N-CA-C	-5.23	106.85	113.18
1	D	41	ALA	N-CA-C	5.15	116.98	111.36
4	H	40	LYS	CB-CA-C	-5.13	110.64	116.54
1	D	42	SER	N-CA-C	5.07	117.70	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	80	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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	2247	0	2096	53	0
1	D	2247	0	2096	88	0
2	B	837	0	803	15	0
2	E	837	0	803	13	0
3	C	77	0	79	1	0
3	F	77	0	79	3	0
4	G	832	0	817	7	0
4	H	813	0	796	31	1
5	A	107	0	0	6	0
5	B	52	0	0	1	0
5	C	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	101	0	0	3	0
5	E	35	0	0	3	0
5	F	4	0	0	0	0
5	G	82	0	0	0	0
5	H	81	0	0	2	0
All	All	8439	0	7569	190	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 12.

All (190) 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:219:ARG:HE	1:D:224:GLN:NE2	1.59	1.00
1:D:63:GLU:O	1:D:67:VAL:HG23	1.61	0.99
1:A:63:GLU:O	1:A:67:VAL:HG23	1.72	0.89
2:E:22:PHE:HD2	4:H:89:MET:HE1	1.38	0.85
1:D:14:ARG:HD2	1:D:19:GLU:O	1.76	0.84
1:A:266:LEU:HD13	1:A:270:LEU:HD13	1.59	0.82
2:B:73:THR:HG22	2:B:75:LYS:H	1.46	0.81
2:B:0:MET:HG2	2:B:1:ILE:H	1.47	0.79
2:E:13:HIS:CD2	4:H:89:MET:HE3	2.19	0.77
1:D:228:THR:HG22	1:D:247:VAL:CG1	2.14	0.77
4:H:68:GLU:H	4:H:68:GLU:CD	1.94	0.76
5:E:106:HOH:O	4:H:89:MET:HE2	1.87	0.74
2:E:13:HIS:NE2	4:H:89:MET:HE3	2.03	0.74
1:D:191:HIS:CE1	1:D:199:ALA:HB1	2.23	0.74
1:D:258:THR:HG22	1:D:273:ARG:HG2	1.68	0.73
1:A:168:LEU:HD22	1:A:172:LEU:HD22	1.72	0.72
2:E:85:VAL:HG13	5:E:101:HOH:O	1.88	0.72
1:A:187:THR:HG22	5:A:392:HOH:O	1.90	0.72
1:D:228:THR:HG22	1:D:247:VAL:HG12	1.72	0.71
1:D:219:ARG:NE	1:D:224:GLN:NE2	2.36	0.71
1:A:63:GLU:O	1:A:67:VAL:CG2	2.38	0.70
1:A:127:LYS:HD2	1:A:132:SER:OG	1.91	0.70
1:A:205:ALA:C	1:A:206:LEU:HD12	2.17	0.69
1:D:20:PRO:HD2	1:D:75:ARG:HD3	1.75	0.69
1:D:65:ARG:HD2	5:D:401:HOH:O	1.93	0.69
1:D:63:GLU:O	1:D:67:VAL:CG2	2.41	0.68
1:D:226:GLN:O	1:D:227:ASP:HB2	1.94	0.67
1:D:67:VAL:HG22	3:F:2:LEU:HD21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:VAL:HG22	3:F:2:LEU:CD2	2.24	0.67
1:A:194:VAL:CG2	1:A:198:GLU:HG3	2.26	0.66
1:A:238:ASP:OD1	1:A:240:THR:HG22	1.97	0.65
1:D:146:LYS:HE3	3:F:8:TYR:O	1.97	0.65
1:A:249:VAL:HG13	1:A:250:PRO:HD2	1.79	0.65
4:H:23:THR:HG22	5:H:204:HOH:O	1.98	0.64
1:D:215:LEU:HD13	1:D:243:LYS:HD3	1.80	0.64
4:H:35:LEU:O	4:H:36:ILE:HD12	1.99	0.63
4:H:35:LEU:C	4:H:36:ILE:HD12	2.23	0.63
1:A:225:THR:C	1:A:227:ASP:H	2.05	0.63
2:B:0:MET:HG2	2:B:1:ILE:N	2.14	0.62
1:A:204:TRP:HB3	1:A:206:LEU:HD11	1.81	0.62
1:D:226:GLN:O	1:D:227:ASP:CB	2.47	0.62
1:A:144:LYS:O	1:A:148:GLU:HG3	2.00	0.62
1:D:219:ARG:HE	1:D:224:GLN:CD	2.08	0.62
1:D:178:THR:HG23	4:H:51:ILE:HD11	1.82	0.62
4:H:76:LYS:HE3	5:H:261:HOH:O	2.00	0.62
1:D:107:TRP:HZ3	1:D:172:LEU:HD13	1.65	0.61
1:D:131:ARG:HD3	1:D:157:ARG:NH2	2.14	0.61
1:D:202:ARG:HD2	1:D:204:TRP:NE1	2.15	0.61
1:D:189:MET:HE1	1:D:274:TRP:HB2	1.82	0.60
4:H:85:ILE:O	4:H:88:TYR:HD2	1.83	0.60
2:E:12:ARG:HD2	4:H:89:MET:CE	2.31	0.60
2:E:22:PHE:CD2	4:H:89:MET:HE1	2.29	0.60
4:H:68:GLU:CD	4:H:68:GLU:N	2.59	0.60
1:D:250:PRO:HB2	1:D:253:GLN:HG3	1.83	0.60
1:A:258:THR:HG23	1:A:260:HIS:NE2	2.18	0.59
2:B:4:THR:OG1	2:B:86:THR:HG21	2.02	0.59
1:A:207:SER:HA	1:A:240:THR:HG21	1.84	0.58
1:A:5:MET:HB2	1:A:168:LEU:HG	1.86	0.57
1:D:162:GLY:O	1:D:165:VAL:HG22	2.05	0.57
1:D:219:ARG:HE	1:D:224:GLN:HE22	1.46	0.57
1:A:194:VAL:HG21	1:A:198:GLU:HG3	1.86	0.56
1:A:207:SER:HA	1:A:240:THR:CG2	2.35	0.56
1:D:49:ALA:O	1:D:52:ILE:HG22	2.05	0.56
2:E:24:ASN:HB3	2:E:65:LEU:HD11	1.88	0.56
1:D:253:GLN:HB3	1:D:256:ARG:CD	2.36	0.55
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.87	0.55
4:G:3:LYS:NZ	4:G:3:LYS:HB2	2.21	0.55
1:D:250:PRO:O	1:D:252:GLY:N	2.40	0.55
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ALA:HB3	1:A:240:THR:HG22	1.90	0.54
1:D:202:ARG:HD2	1:D:204:TRP:CE2	2.42	0.54
1:A:70:HIS:O	1:A:73:THR:HG22	2.08	0.54
4:G:57:THR:OG1	4:G:59:ASP:OD1	2.23	0.53
4:H:27:LYS:HG2	4:H:47:ALA:HB2	1.90	0.53
1:A:45:MET:HE2	1:A:67:VAL:HG22	1.90	0.53
1:A:40:ALA:HB3	5:A:379:HOH:O	2.09	0.53
4:H:23:THR:HG23	4:H:49:TYR:CE1	2.43	0.53
1:A:168:LEU:HD22	1:A:172:LEU:CD2	2.39	0.53
1:D:266:LEU:HD13	1:D:270:LEU:HD13	1.90	0.52
1:A:49:ALA:O	1:A:52:ILE:HG22	2.08	0.52
1:A:258:THR:HG22	5:A:374:HOH:O	2.08	0.52
1:D:191:HIS:NE2	1:D:199:ALA:HB1	2.25	0.52
1:D:177:GLU:HB3	4:H:51:ILE:HD13	1.92	0.51
1:D:191:HIS:CE1	1:D:199:ALA:CB	2.93	0.51
1:D:193:ALA:C	1:D:195:SER:H	2.19	0.51
1:D:219:ARG:HA	1:D:256:ARG:O	2.10	0.51
1:D:138:MET:HE3	1:D:141:GLN:HB2	1.94	0.50
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.50
1:D:105:SER:O	1:D:106:ASP:HB2	2.11	0.50
1:D:214:THR:HB	1:D:262:GLN:HB2	1.93	0.50
1:A:45:MET:HE2	1:A:67:VAL:CG2	2.40	0.50
4:H:36:ILE:HD13	4:H:65:PHE:CE2	2.46	0.50
1:D:110:LEU:HB3	1:D:111:ARG:NH1	2.27	0.49
4:H:35:LEU:C	4:H:35:LEU:HD12	2.38	0.49
1:D:191:HIS:HD2	1:D:201:LEU:HD21	1.77	0.49
1:D:253:GLN:HB3	1:D:256:ARG:HD2	1.93	0.49
1:D:17:ARG:HH11	1:D:17:ARG:HG3	1.77	0.48
1:A:249:VAL:HG13	1:A:257:TYR:CE2	2.48	0.48
1:A:214:THR:HB	1:A:262:GLN:HB2	1.95	0.48
1:D:202:ARG:NH1	1:D:244:TRP:CZ3	2.81	0.48
4:H:59:ASP:OD1	4:H:76:LYS:HG3	2.13	0.48
1:D:177:GLU:CB	4:H:51:ILE:HD13	2.43	0.48
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.96	0.48
1:D:104:GLY:O	1:D:106:ASP:O	2.32	0.48
2:B:97:ARG:O	2:B:97:ARG:HG3	2.14	0.48
1:A:73:THR:HG21	5:A:310:HOH:O	2.14	0.47
1:A:204:TRP:HB3	1:A:206:LEU:CD1	2.43	0.47
1:D:97:ARG:NH2	5:D:361:HOH:O	2.39	0.47
4:H:82:MET:HA	4:H:85:ILE:HD12	1.96	0.47
1:D:189:MET:HE3	1:D:201:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:THR:C	1:A:227:ASP:N	2.72	0.47
1:A:266:LEU:HD22	1:A:270:LEU:HD11	1.95	0.47
4:G:3:LYS:HG3	4:G:4:VAL:N	2.30	0.47
4:G:35:LEU:C	4:G:35:LEU:HD12	2.39	0.47
2:B:73:THR:HG22	2:B:74:GLU:N	2.29	0.46
2:E:4:THR:HG22	5:E:103:HOH:O	2.15	0.46
4:H:2:LYS:HG2	4:H:2:LYS:O	2.16	0.46
1:D:177:GLU:OE2	4:H:42:LYS:HE3	2.16	0.46
1:D:224:GLN:NE2	1:D:224:GLN:HA	2.28	0.46
1:D:274:TRP:O	1:D:275:GLU:HB2	2.15	0.46
1:D:107:TRP:CZ3	1:D:172:LEU:HD13	2.49	0.46
1:D:202:ARG:HH11	1:D:202:ARG:HG3	1.80	0.46
2:E:51:HIS:HA	2:E:65:LEU:O	2.16	0.45
4:H:33:GLU:CD	4:H:67:GLY:H	2.24	0.45
1:A:194:VAL:HG22	1:A:198:GLU:O	2.16	0.45
2:B:51:HIS:HA	2:B:65:LEU:O	2.17	0.45
1:D:221:GLY:O	1:D:222:GLU:HB2	2.16	0.45
1:D:266:LEU:HD22	1:D:270:LEU:CD1	2.45	0.45
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.51	0.45
1:D:107:TRP:CD1	1:D:169:ARG:NH2	2.85	0.45
1:D:218:GLN:O	1:D:257:TYR:HA	2.17	0.45
1:D:253:GLN:HB3	1:D:256:ARG:NE	2.31	0.45
1:A:11:SER:HB3	1:A:95:VAL:CG1	2.47	0.45
1:D:191:HIS:HD2	1:D:201:LEU:CD2	2.30	0.45
1:D:81:LEU:HD13	1:D:118:TYR:CD1	2.52	0.45
1:A:258:THR:OG1	1:A:271:THR:HG23	2.18	0.44
1:D:271:THR:C	1:D:272:LEU:HD22	2.42	0.44
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.99	0.44
1:D:214:THR:C	1:D:215:LEU:HD12	2.42	0.44
1:D:224:GLN:O	1:D:226:GLN:N	2.50	0.44
1:A:272:LEU:HD22	1:A:272:LEU:N	2.32	0.44
2:B:9:VAL:HG13	5:B:114:HOH:O	2.17	0.44
1:A:35:ARG:HD3	1:A:35:ARG:C	2.42	0.44
1:D:224:GLN:C	1:D:226:GLN:H	2.25	0.44
2:E:12:ARG:HD2	4:H:89:MET:HE1	1.98	0.44
2:B:73:THR:HG22	2:B:75:LYS:N	2.25	0.44
1:A:214:THR:HG22	5:A:339:HOH:O	2.17	0.44
2:B:31:HIS:ND1	2:B:32:PRO:HA	2.33	0.44
1:A:204:TRP:CZ3	2:B:99:MET:HB3	2.53	0.43
1:A:207:SER:C	1:A:240:THR:OG1	2.61	0.43
1:D:206:LEU:HD23	1:D:242:GLN:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ASP:O	2:B:97:ARG:C	2.61	0.43
1:D:219:ARG:CG	1:D:224:GLN:OE1	2.67	0.43
2:E:36:GLU:HB2	2:E:83:ASN:HB3	2.01	0.43
1:D:51:TRP:CZ2	1:D:179:LEU:HD11	2.54	0.43
1:A:178:THR:CG2	4:G:49:TYR:OH	2.67	0.43
1:D:14:ARG:HG2	5:D:368:HOH:O	2.17	0.43
1:A:250:PRO:HG2	1:A:253:GLN:HB2	2.00	0.43
1:D:189:MET:CE	1:D:201:LEU:HD22	2.49	0.43
1:A:73:THR:OG1	3:C:7:VAL:O	2.24	0.42
1:D:248:VAL:O	1:D:248:VAL:HG13	2.18	0.42
1:A:186:LYS:HE2	4:G:95:LEU:HD22	2.02	0.42
4:H:39:HIS:HB3	4:H:48:VAL:HG11	2.01	0.42
1:A:106:ASP:CG	1:A:108:ARG:HE	2.28	0.42
1:D:219:ARG:HG3	1:D:224:GLN:OE1	2.19	0.42
1:D:177:GLU:OE2	4:H:50:ALA:HA	2.20	0.42
4:G:32:HIS:HB3	4:G:65:PHE:O	2.20	0.42
1:A:267:PRO:HB2	1:A:268:LYS:HE3	2.00	0.42
1:A:42:SER:O	1:A:43:GLN:HB2	2.19	0.42
1:D:33:PHE:CD1	1:D:34:VAL:HG13	2.55	0.42
1:D:189:MET:CE	1:D:274:TRP:HB2	2.50	0.41
1:A:73:THR:HG23	5:A:377:HOH:O	2.19	0.41
1:A:206:LEU:HD12	1:A:206:LEU:N	2.35	0.41
1:D:138:MET:HE3	1:D:138:MET:O	2.20	0.41
1:D:181:ARG:NH1	1:D:183:ASP:OD2	2.45	0.41
1:D:191:HIS:NE2	1:D:199:ALA:CB	2.84	0.41
1:D:189:MET:HE2	1:D:274:TRP:HE3	1.85	0.41
1:D:196:ASP:HB3	1:D:197:HIS:H	1.58	0.41
4:H:80:TYR:CD2	4:H:80:TYR:C	2.99	0.41
1:A:219:ARG:C	1:A:221:GLY:N	2.79	0.41
1:D:215:LEU:HD12	1:D:215:LEU:N	2.35	0.41
1:D:224:GLN:C	1:D:226:GLN:N	2.78	0.41
1:D:193:ALA:HA	1:D:199:ALA:HA	2.02	0.41
4:H:23:THR:CG2	4:H:49:TYR:HE1	2.34	0.41
1:D:2:SER:HB2	1:D:103:VAL:O	2.21	0.40
1:D:253:GLN:NE2	1:D:256:ARG:NH1	2.69	0.40
1:A:88:SER:N	2:E:36:GLU:OE2	2.35	0.40
4:H:88:TYR:CD1	4:H:89:MET:N	2.90	0.40
1:D:111:ARG:HD2	1:D:113:TYR:OH	2.21	0.40
1:D:219:ARG:HG2	1:D:224:GLN:CD	2.46	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:H:85:ILE:CD1	4:H:85:ILE:CD1[8_554]	2.18	0.02

### 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	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
1	D	273/275 (99%)	257 (94%)	11 (4%)	5 (2%)	6	1
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	E	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
4	G	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
4	H	95/100 (95%)	94 (99%)	1 (1%)	0	100	100
All	All	948/968 (98%)	920 (97%)	23 (2%)	5 (0%)	24	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	225	THR
1	D	251	SER
1	D	194	VAL
1	D	222	GLU
1	D	252	GLY

#### 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	231/231 (100%)	220 (95%)	11 (5%)	23	12
1	D	231/231 (100%)	218 (94%)	13 (6%)	19	8
2	B	95/95 (100%)	95 (100%)	0	100	100
2	E	95/95 (100%)	95 (100%)	0	100	100
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	1
3	F	8/8 (100%)	7 (88%)	1 (12%)	4	1
4	G	92/92 (100%)	89 (97%)	3 (3%)	33	24
4	H	90/92 (98%)	88 (98%)	2 (2%)	45	40
All	All	850/852 (100%)	819 (96%)	31 (4%)	31	21

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

Mol	Chain	Res	Type
1	A	31	THR
1	A	35	ARG
1	A	67	VAL
1	A	98	MET
1	A	110	LEU
1	A	141	GLN
1	A	168	LEU
1	A	172	LEU
1	A	178	THR
1	A	226	GLN
1	A	240	THR
3	C	2	LEU
1	D	14	ARG
1	D	67	VAL
1	D	72	GLN
1	D	110	LEU
1	D	127	LYS
1	D	128	GLU
1	D	130	LEU
1	D	156	LEU
1	D	169	ARG
1	D	181	ARG
1	D	197	HIS
1	D	223	ASP

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Mol	Chain	Res	Type
1	D	226	GLN
3	F	2	LEU
4	G	3	LYS
4	G	25	LEU
4	G	68	GLU
4	H	68	GLU
4	H	74	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	141	GLN
1	A	218	GLN
1	A	262	GLN
1	D	72	GLN
1	D	115	GLN
1	D	191	HIS
1	D	218	GLN
1	D	224	GLN
1	D	253	GLN
4	G	20	ASN
4	G	66	GLN
4	G	92	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 oligosaccharides 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	275/275 (100%)	0.81	41 (14%) 5 6	19, 33, 65, 96	0
1	D	275/275 (100%)	0.89	54 (19%) 3 3	17, 30, 83, 105	0
2	B	100/100 (100%)	0.82	13 (13%) 7 8	19, 33, 57, 87	1 (1%)
2	E	100/100 (100%)	0.70	9 (9%) 15 17	21, 36, 61, 81	0
3	C	9/9 (100%)	0.59	1 (11%) 10 12	25, 26, 29, 46	0
3	F	9/9 (100%)	1.22	3 (33%) 1 0	20, 29, 40, 49	0
4	G	99/100 (99%)	0.29	7 (7%) 22 25	12, 24, 48, 81	2 (2%)
4	H	97/100 (97%)	0.63	10 (10%) 12 13	17, 26, 56, 100	1 (1%)
All	All	964/968 (99%)	0.75	138 (14%) 6 7	12, 30, 69, 105	4 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	88	TYR	7.3
1	D	195	SER	6.4
1	D	194	VAL	6.4
4	H	4	VAL	5.8
1	D	225	THR	5.7
1	A	138	MET	5.3
1	A	197	HIS	5.2
1	D	193	ALA	5.1
2	B	0	MET	5.1
1	D	251	SER	5.1
1	D	274	TRP	4.9
1	A	275	GLU	4.9
1	D	197	HIS	4.9
2	E	0	MET	4.8
1	D	196	ASP	4.6
1	D	138	MET	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	219	ARG	4.4
1	A	136	ALA	4.4
1	A	225	THR	4.3
1	A	274	TRP	4.3
1	D	1	GLY	4.3
4	G	3	LYS	4.3
1	D	17	ARG	4.2
2	B	1	ILE	4.1
4	H	3	LYS	4.1
1	D	247	VAL	4.1
2	E	1	ILE	4.1
1	A	228	THR	4.1
4	H	2	LYS	4.1
3	C	5	TYR	4.0
1	D	270	LEU	4.0
1	A	195	SER	3.9
1	D	221	GLY	3.9
4	G	100	LYS	3.8
1	D	199	ALA	3.8
4	H	70	ARG	3.8
4	G	2	LYS	3.8
1	A	1	GLY	3.7
1	A	224	GLN	3.7
1	D	255	GLN	3.5
1	D	223	ASP	3.5
4	G	4	VAL	3.4
1	D	216	THR	3.4
1	A	251	SER	3.4
1	D	220	ASP	3.4
1	D	191	HIS	3.3
1	A	90	ALA	3.3
1	D	227	ASP	3.3
1	A	249	VAL	3.2
1	D	215	LEU	3.2
4	G	81	GLU	3.2
1	D	116	TYR	3.2
1	A	194	VAL	3.2
1	D	230	LEU	3.2
2	B	48	LYS	3.2
1	A	221	GLY	3.1
1	A	258	THR	3.1
4	H	98	PRO	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	107	TRP	3.1
1	A	145	HIS	3.1
4	H	85	ILE	3.1
1	D	267	PRO	3.1
1	A	256	ARG	3.0
1	A	227	ASP	3.0
1	D	273	ARG	3.0
1	D	272	LEU	3.0
1	A	187	THR	3.0
1	D	228	THR	3.0
1	A	223	ASP	2.9
2	E	48	LYS	2.9
1	D	256	ARG	2.9
1	D	105	SER	2.9
1	D	192	HIS	2.9
1	D	248	VAL	2.9
4	G	88	TYR	2.9
2	B	75	LYS	2.8
4	H	68	GLU	2.8
3	F	7	VAL	2.8
1	A	220	ASP	2.8
1	A	230	LEU	2.8
3	F	6	PRO	2.8
2	E	99	MET	2.7
1	A	222	GLU	2.7
1	D	257	TYR	2.7
1	A	151	HIS	2.7
2	B	74	GLU	2.6
1	D	226	GLN	2.6
3	F	5	TYR	2.6
1	D	200	THR	2.6
2	E	75	LYS	2.6
1	D	169	ARG	2.6
1	D	141	GLN	2.5
2	E	85	VAL	2.5
2	B	86	THR	2.5
1	A	219	ARG	2.5
1	D	224	GLN	2.5
1	A	154	GLU	2.5
1	D	222	GLU	2.5
1	A	270	LEU	2.5
1	A	226	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	106	ASP	2.5
2	B	49	VAL	2.5
1	D	254	GLU	2.4
1	D	136	ALA	2.4
2	B	47	GLU	2.4
2	E	74	GLU	2.4
1	D	86	ASN	2.4
1	D	104	GLY	2.4
1	A	196	ASP	2.3
1	A	18	GLY	2.3
2	B	96	ASP	2.3
1	A	135	ALA	2.3
4	H	41	ASP	2.3
1	D	249	VAL	2.3
2	B	88	SER	2.2
1	A	268	LYS	2.2
2	B	3	ARG	2.2
1	D	201	LEU	2.2
1	D	275	GLU	2.2
1	D	229	GLU	2.2
4	G	5	GLU	2.2
1	A	247	VAL	2.2
1	A	15	PRO	2.2
1	A	264	GLU	2.1
1	A	82	ARG	2.1
1	A	73	THR	2.1
2	E	43	GLY	2.1
1	D	268	LYS	2.1
2	E	47	GLU	2.1
4	H	18	GLU	2.1
1	D	218	GLN	2.1
1	A	17	ARG	2.1
2	B	92	ILE	2.0
1	D	260	HIS	2.0
1	D	253	GLN	2.0
2	B	85	VAL	2.0
1	A	108	ARG	2.0
1	A	193	ALA	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.