



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 10, 2022 – 09:13 PM EST

PDB ID : 1LP9  
Title : Xenoreactive complex AHIII 12.2 TCR bound to p1049/HLA-A2.1  
Authors : Buslepp, J.; Wang, H.; Biddison, W.E.; Appella, E.; Collins, E.J.  
Deposited on : 2002-05-07  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

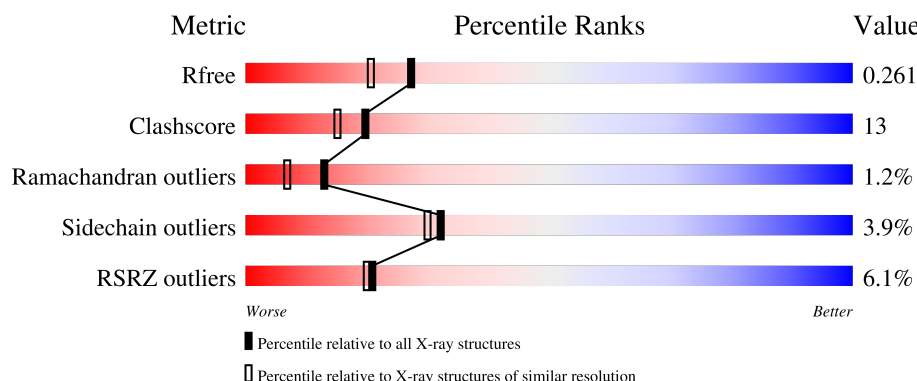
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	<div> <div>3%</div> <div>81%</div> <div>13%</div> <div>..</div> </div>
1	H	275	<div> <div>5%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
2	B	100	<div> <div>3%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
2	I	100	<div> <div>4%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
3	C	9	<div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	J	9	<div><div></div><div>11%</div><div>100%</div></div>
4	E	194	<div><div></div><div>12%</div><div>63%</div><div>28%</div><div>8%</div><div></div></div>
4	L	194	<div><div></div><div>14%</div><div>68%</div><div>21%</div><div>7%</div><div>5%</div><div></div></div>
5	F	238	<div><div></div><div>4%</div><div>72%</div><div>24%</div><div></div><div></div></div>
5	M	238	<div><div></div><div>3%</div><div>79%</div><div>15%</div><div>5%</div><div></div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13552 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
1	A	275	Total	C	N	O	S	14	0	0
			2247	1403	409	426	9			
1	H	275	Total	C	N	O	S	18	0	0
			2247	1403	409	426	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	9	0	0
			837	533	141	159	4			
2	I	100	Total	C	N	O	S	5	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
I	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called self-peptide P1049.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			76	56	10	10			
3	J	9	Total	C	N	O	0	0	0
			76	56	10	10			

- Molecule 4 is a protein called T-cell Receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	194	Total	C	N	O	S	102	0	0
			1521	965	245	302	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	194	Total	C	N	O	S	96	0	0
			1521	965	245	302	9			

- Molecule 5 is a protein called T-cell Receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	237	Total	C	N	O	S	27	0	0
			1887	1192	331	359	5			
5	M	237	Total	C	N	O	S	25	0	0
			1887	1192	331	359	5			

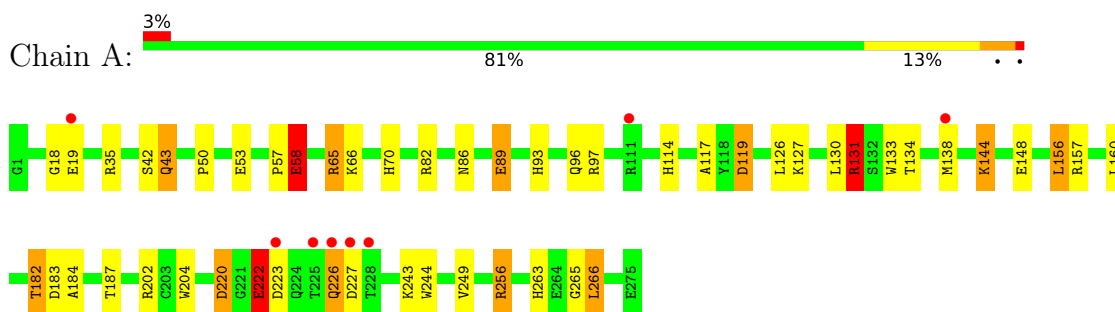
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total	O	0	0
			79	79		
6	B	20	Total	O	0	0
			20	20		
6	C	3	Total	O	0	0
			3	3		
6	E	47	Total	O	0	0
			47	47		
6	F	46	Total	O	0	0
			46	46		
6	H	64	Total	O	0	0
			64	64		
6	I	28	Total	O	0	0
			28	28		
6	J	2	Total	O	0	0
			2	2		
6	L	53	Total	O	0	0
			53	53		
6	M	74	Total	O	0	0
			74	74		

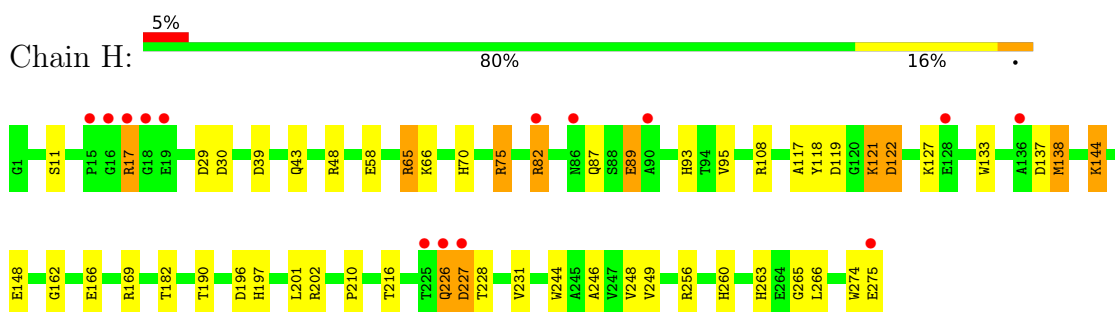
### 3 Residue-property plots [i](#)

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.

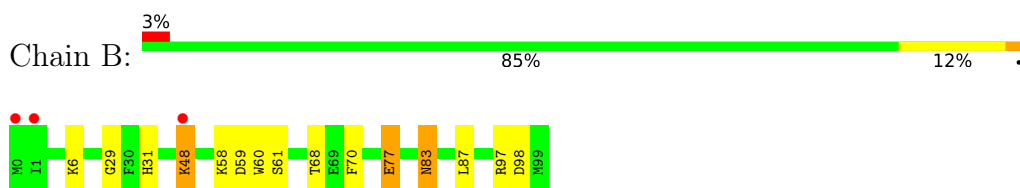
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



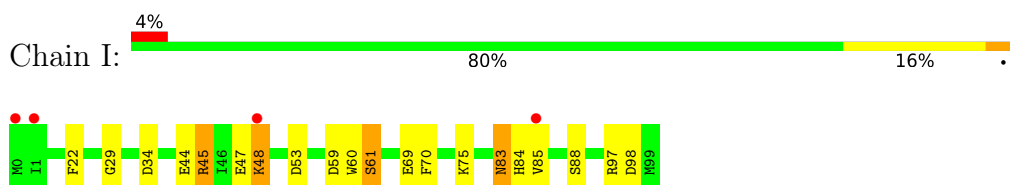
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain




- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



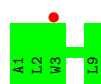
- Molecule 3: self-peptide P1049

Chain C:  89% 11%



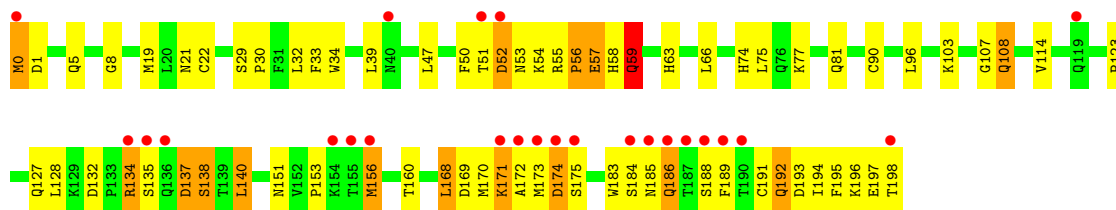
- Molecule 3: self-peptide P1049

Chain J:  11% 100%



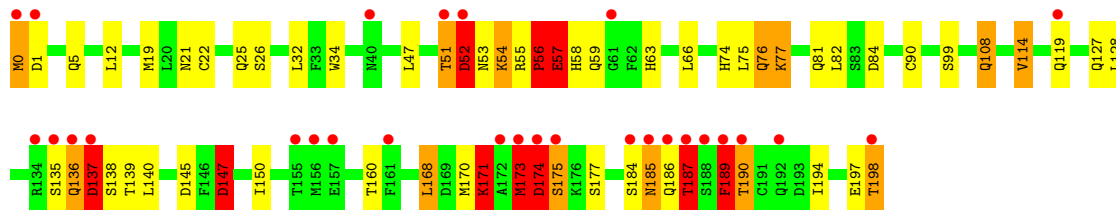
- Molecule 4: T-cell Receptor alpha chain

Chain E:  12% 63% 28% 8%



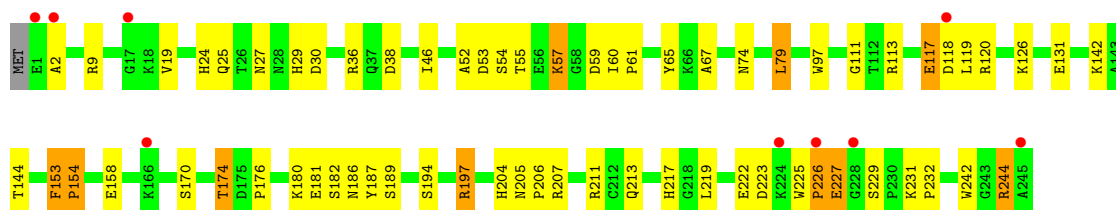
- Molecule 4: T-cell Receptor alpha chain

Chain L:  14% 68% 21% 7% 5%




- Molecule 5: T-cell Receptor beta chain

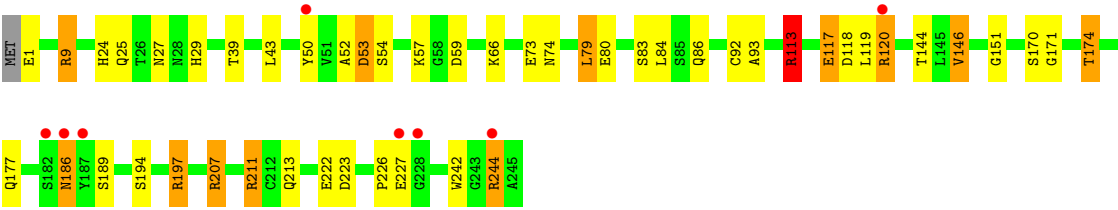
Chain F:  4% 72% 24%



- Molecule 5: T-cell Receptor beta chain

Chain M:  3% 79% 15% 5%







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.71Å 84.47Å 121.34Å 90.00° 92.13° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.00) 100.0 (29.96-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.219 , 0.253 0.230 , 0.261	Depositor DCC
$R_{free}$ test set	6421 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	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 45.70 % 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 1.2719e-04. 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	2.22	13/2312 (0.6%)	1.24	20/3137 (0.6%)
1	H	1.24	9/2312 (0.4%)	2.48	26/3137 (0.8%)
2	B	1.93	4/860 (0.5%)	1.59	7/1162 (0.6%)
2	I	3.59	7/860 (0.8%)	0.96	7/1162 (0.6%)
3	C	0.67	0/80	0.73	0/108
3	J	0.64	0/80	0.67	0/108
4	E	2.39	21/1557 (1.3%)	1.67	35/2112 (1.7%)
4	L	1.78	20/1557 (1.3%)	1.94	38/2112 (1.8%)
5	F	2.34	17/1943 (0.9%)	2.17	24/2644 (0.9%)
5	M	2.36	13/1943 (0.7%)	2.47	24/2644 (0.9%)
All	All	2.19	104/13504 (0.8%)	1.96	181/18326 (1.0%)

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	4
1	H	0	2
2	B	0	1
4	E	1	4
4	L	0	7
5	F	0	4
5	M	0	4
All	All	1	26

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	GLU	CG-CD	87.36	2.83	1.51
2	I	44	GLU	CD-OE1	68.60	2.01	1.25
2	I	44	GLU	CD-OE2	61.19	1.93	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	117	GLU	CG-CD	59.87	2.41	1.51
5	F	222	GLU	CG-CD	48.99	2.25	1.51

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	17	ARG	NE-CZ-NH1	-101.59	69.50	120.30
5	M	207	ARG	NE-CZ-NH1	-65.69	87.46	120.30
5	M	207	ARG	NE-CZ-NH2	-56.78	91.91	120.30
1	H	17	ARG	NE-CZ-NH2	51.09	145.84	120.30
5	F	207	ARG	NE-CZ-NH1	-50.50	95.05	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	57	GLU	CA

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain
1	A	222	GLU	Sidechain
1	A	58	GLU	Sidechain
1	A	65	ARG	Sidechain
2	B	77	GLU	Sidechain

## 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	2247	0	2096	49	0
1	H	2247	0	2096	38	4
2	B	837	0	803	11	0
2	I	837	0	803	16	1
3	C	76	0	76	1	0
3	J	76	0	76	0	0
4	E	1521	0	1473	63	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1521	0	1475	63	0
5	F	1887	0	1790	58	0
5	M	1887	0	1790	45	1
6	A	79	0	0	7	0
6	B	20	0	0	4	0
6	C	3	0	0	0	0
6	E	47	0	0	8	0
6	F	46	0	0	4	0
6	H	64	0	0	3	0
6	I	28	0	0	9	0
6	J	2	0	0	0	0
6	L	53	0	0	9	0
6	M	74	0	0	14	0
All	All	13552	0	12478	316	5

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 13.

The worst 5 of 316 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)
5:M:244:ARG:HG2	6:M:306:HOH:O	1.35	1.24
1:A:138:MET:HG3	6:A:336:HOH:O	1.39	1.19
4:L:99:SER:CB	6:L:250:HOH:O	1.87	1.19
4:L:0:MET:CE	4:L:1:ASP:H	1.56	1.18
5:M:244:ARG:CG	6:M:306:HOH:O	1.84	1.18

All (5) 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:E:198:THR:OG1	1:H:108:ARG:NE[2_645]	1.92	0.28
4:E:198:THR:O	1:H:169:ARG:NH1[2_645]	2.03	0.17
1:H:226:GLN:NE2	2:I:75:LYS:NZ[2_546]	2.15	0.05
4:E:198:THR:O	1:H:169:ARG:NH2[2_645]	2.16	0.04
4:E:59:GLN:NE2	5:M:84:LEU:CB[1_545]	2.19	0.01

## 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	273/275 (99%)	266 (97%)	6 (2%)	1 (0%)	34	30
1	H	273/275 (99%)	269 (98%)	4 (2%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	I	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	J	7/9 (78%)	7 (100%)	0	0	100	100
4	E	192/194 (99%)	170 (88%)	17 (9%)	5 (3%)	5	2
4	L	192/194 (99%)	172 (90%)	9 (5%)	11 (6%)	1	0
5	F	235/238 (99%)	223 (95%)	10 (4%)	2 (1%)	17	11
5	M	235/238 (99%)	225 (96%)	9 (4%)	1 (0%)	34	30
All	All	1610/1632 (99%)	1533 (95%)	57 (4%)	20 (1%)	13	7

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	39	LEU
4	E	52	ASP
4	E	56	PRO
5	F	154	PRO
4	L	51	THR

### 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	231/231 (100%)	226 (98%)	5 (2%)	52	55
1	H	231/231 (100%)	227 (98%)	4 (2%)	60	65
2	B	95/95 (100%)	93 (98%)	2 (2%)	53	57
2	I	95/95 (100%)	92 (97%)	3 (3%)	39	38
3	C	7/7 (100%)	7 (100%)	0	100	100
3	J	7/7 (100%)	7 (100%)	0	100	100
4	E	177/177 (100%)	164 (93%)	13 (7%)	14	9
4	L	177/177 (100%)	161 (91%)	16 (9%)	9	6
5	F	204/206 (99%)	199 (98%)	5 (2%)	47	49
5	M	204/206 (99%)	197 (97%)	7 (3%)	37	36
All	All	1428/1432 (100%)	1373 (96%)	55 (4%)	32	30

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	266	LEU
4	L	57	GLU
5	M	244	ARG
5	M	54	SER
2	I	70	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	89	GLN
5	M	25	GLN
4	L	5	GLN
4	L	74	HIS
5	M	86	GLN

### 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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	59:GLN	C	61:GLY	N	0.94

## 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%)	0.16	8 (2%) 51 50	9, 15, 20, 24	8 (2%)
1	H	275/275 (100%)	0.15	14 (5%) 28 27	11, 15, 20, 26	11 (4%)
2	B	100/100 (100%)	-0.05	3 (3%) 50 49	11, 15, 22, 25	6 (6%)
2	I	100/100 (100%)	-0.05	4 (4%) 38 37	11, 15, 20, 25	3 (3%)
3	C	9/9 (100%)	1.10	0 100 100	13, 13, 14, 15	0
3	J	9/9 (100%)	1.27	1 (11%) 5 4	13, 14, 15, 16	0
4	E	187/194 (96%)	0.66	24 (12%) 3 3	10, 15, 21, 29	19 (10%)
4	L	187/194 (96%)	0.71	28 (14%) 2 2	10, 15, 21, 31	22 (11%)
5	F	237/238 (99%)	0.21	9 (3%) 40 39	11, 15, 19, 23	11 (4%)
5	M	237/238 (99%)	0.04	8 (3%) 45 44	11, 15, 19, 24	13 (5%)
All	All	1616/1632 (99%)	0.25	99 (6%) 21 20	9, 15, 20, 31	93 (5%)

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	52	ASP	8.6
4	E	187	THR	8.5
4	L	188	SER	8.4
4	E	190	THR	8.0
4	E	188	SER	7.9

### 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.