



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:40 pm BST

PDB ID : 1ZHB  
Title : Crystal Structure Of The Murine Class I Major Histocompatibility Complex Of H-2Db, B2-Microglobulin, and a 9-Residue Peptide Derived from rat dopamine beta-monooxygenase  
Authors : Sandalova, T.; Michaelsson, J.; Harris, R.A.; Odeberg, J.; Schneider, G.; Karre, K.; Achour, A.  
Deposited on : 2005-04-25  
Resolution : 2.70 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

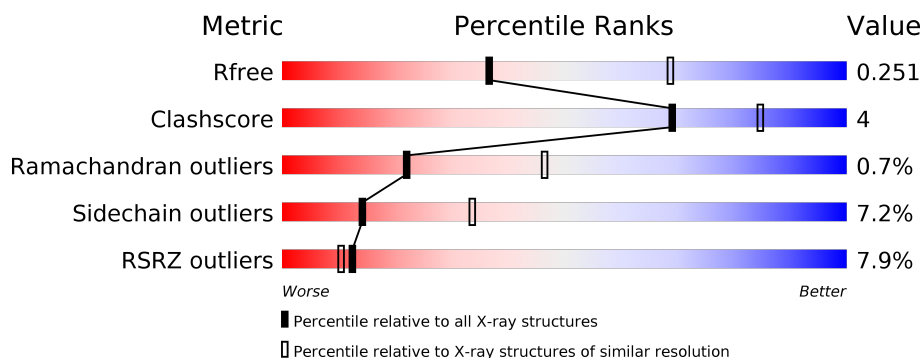
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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>5%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>..</div> </div> </div>
1	D	276	<div> <div>13%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	G	276	<div> <div>13%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	J	276	<div> <div>11%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </div> </div>
2	B	99	<div> <div></div> <div> <div></div> <div>86%</div> <div>11%</div> <div>.</div> </div> </div>
2	E	99	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	99	 3% 86% 12%
2	K	99	 % 84% 16%
3	C	9	 78% 22%
3	F	9	 100%
3	I	9	 78% 22%
3	L	9	 89% 11%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12661 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	D	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	G	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	J	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	E	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	H	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	K	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			

- Molecule 3 is a protein called 9-mer peptide from Dopamine beta-monooxygenase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			74	51	11	12			
3	F	9	Total	C	N	O	0	0	0
			74	51	11	12			
3	I	9	Total	C	N	O	0	0	0
			74	51	11	12			
3	L	9	Total	C	N	O	0	0	0
			74	51	11	12			

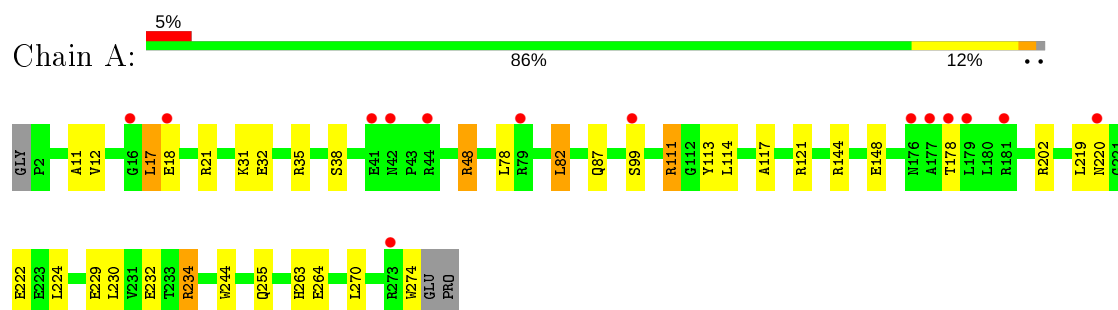
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total 21	O 21	0	0
4	B	7	Total 7	O 7	0	0
4	C	2	Total 2	O 2	0	0
4	D	16	Total 16	O 16	0	0
4	E	9	Total 9	O 9	0	0
4	F	1	Total 1	O 1	0	0
4	G	15	Total 15	O 15	0	0
4	H	10	Total 10	O 10	0	0
4	J	19	Total 19	O 19	0	0
4	K	7	Total 7	O 7	0	0
4	L	2	Total 2	O 2	0	0

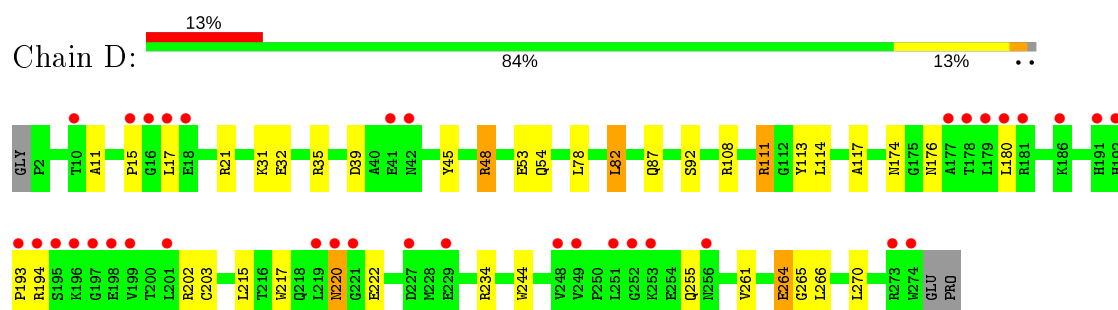
### 3 Residue-property plots [i](#)

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.

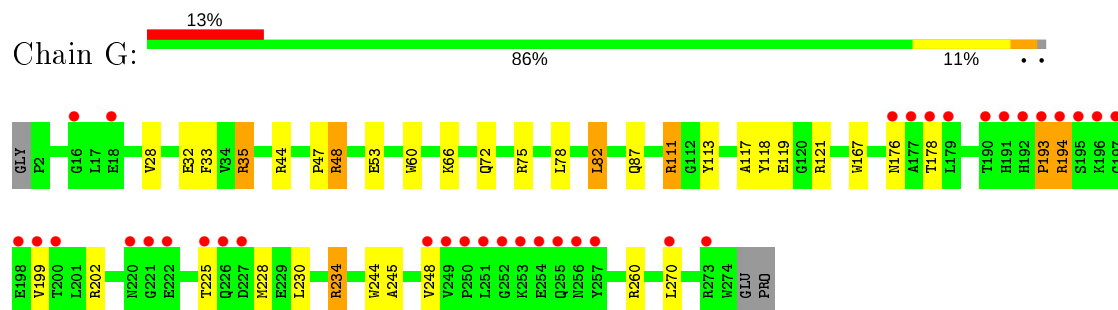
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



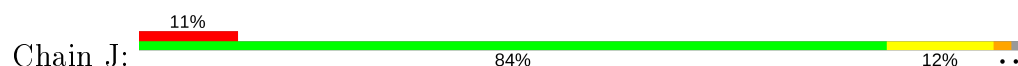
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

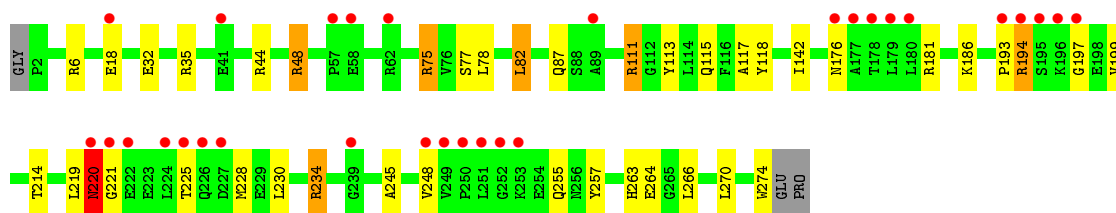


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

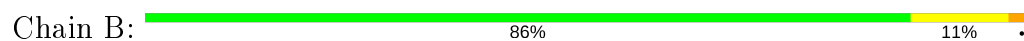


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

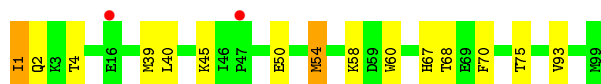
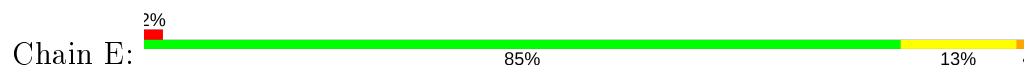




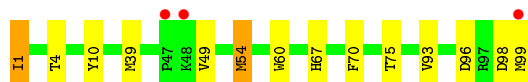
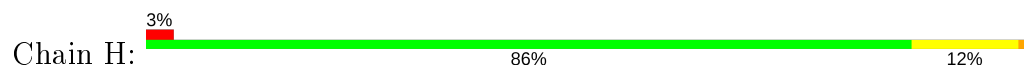
- Molecule 2: Beta-2-microglobulin



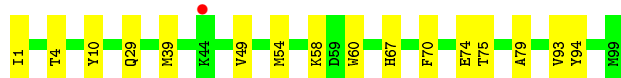
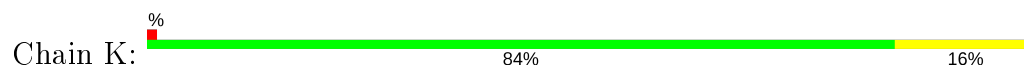
- Molecule 2: Beta-2-microglobulin



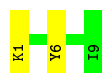
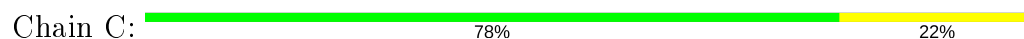
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: 9-mer peptide from Dopamine beta-monooxygenase




- Molecule 3: 9-mer peptide from Dopamine beta-monooxygenase



There are no outlier residues recorded for this chain.

- Molecule 3: 9-mer peptide from Dopamine beta-monooxygenase

Chain I:  78% 22%



- Molecule 3: 9-mer peptide from Dopamine beta-monooxygenase

Chain L:  89% 11%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.06 Å 122.72 Å 99.40 Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	24.92 – 2.70 24.91 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.92-2.70) 93.4 (24.91-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.90 (at 2.68 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.225 , 0.262 0.240 , 0.251	Depositor DCC
$R_{free}$ test set	2231 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12661	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.34% 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	0.71	1/2310 (0.0%)	0.74	1/3136 (0.0%)
1	D	0.66	0/2310	0.74	0/3136
1	G	0.68	0/2310	0.73	1/3136 (0.0%)
1	J	0.64	0/2310	0.70	0/3136
2	B	0.78	1/846 (0.1%)	0.73	0/1147
2	E	0.71	0/846	0.68	0/1147
2	H	0.72	0/846	0.70	0/1147
2	K	0.72	0/846	0.70	0/1147
3	C	0.67	0/76	0.80	0/102
3	F	0.81	0/76	0.77	0/102
3	I	0.76	0/76	0.89	0/102
3	L	0.89	0/76	0.90	0/102
All	All	0.69	2/12928 (0.0%)	0.73	2/17540 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	74	GLU	CG-CD	6.10	1.61	1.51
1	A	232	GLU	CG-CD	5.54	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	121	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	234	ARG	NE-CZ-NH1	5.62	123.11	120.30

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	2244	0	2118	14	0
1	D	2244	0	2118	16	0
1	G	2244	0	2118	21	0
1	J	2244	0	2118	20	0
2	B	820	0	796	6	0
2	E	820	0	796	6	0
2	H	820	0	796	13	0
2	K	820	0	796	6	0
3	C	74	0	78	0	0
3	F	74	0	78	0	0
3	I	74	0	78	2	0
3	L	74	0	78	1	0
4	A	21	0	0	0	0
4	B	7	0	0	0	0
4	C	2	0	0	0	0
4	D	16	0	0	0	0
4	E	9	0	0	0	0
4	F	1	0	0	0	0
4	G	15	0	0	0	0
4	H	10	0	0	0	0
4	J	19	0	0	1	0
4	K	7	0	0	0	0
4	L	2	0	0	0	0
All	All	12661	0	11968	90	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 4.

All (90) 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:264:GLU:O	1:D:266:LEU:N	2.12	0.82
2:B:39:MET:HE1	2:B:67:HIS:HA	1.67	0.77
2:H:96:ASP:CB	2:H:99:MET:C	2.56	0.74
2:H:96:ASP:HB3	2:H:99:MET:C	2.09	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:ARG:HD2	1:G:48:ARG:HD2	1.73	0.71
1:J:32:GLU:OE2	1:J:48:ARG:HD2	1.91	0.70
2:H:1:ILE:O	2:H:1:ILE:HG23	1.90	0.69
1:J:111:ARG:HD2	1:J:113:TYR:CZ	2.27	0.68
1:J:87:GLN:NE2	1:J:118:TYR:OH	2.24	0.66
1:A:17:LEU:HG	1:A:18:GLU:H	1.63	0.64
2:H:96:ASP:CG	2:H:99:MET:C	2.58	0.62
1:A:263:HIS:ND1	1:A:264:GLU:O	2.34	0.61
1:D:32:GLU:OE2	1:D:48:ARG:HD2	2.01	0.61
2:H:96:ASP:CG	2:H:99:MET:H	2.03	0.60
1:A:35:ARG:NH2	2:B:54:MET:O	2.34	0.59
1:G:32:GLU:OE2	1:G:48:ARG:HD2	2.02	0.58
1:G:87:GLN:NE2	1:G:118:TYR:OH	2.25	0.58
1:D:111:ARG:HD2	1:D:113:TYR:CZ	2.38	0.58
1:A:111:ARG:HD2	1:A:113:TYR:CZ	2.39	0.57
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.39	0.57
2:E:1:ILE:O	2:E:1:ILE:HG23	2.05	0.56
2:B:1:ILE:O	2:B:1:ILE:HG23	2.05	0.56
1:G:35:ARG:NH2	2:H:54:MET:O	2.40	0.55
1:G:82:LEU:HA	1:G:87:GLN:HE21	1.71	0.55
1:G:111:ARG:HD2	1:G:113:TYR:CZ	2.42	0.55
1:D:15:PRO:HD3	1:D:92:SER:OG	2.07	0.54
1:D:35:ARG:NH2	2:E:54:MET:O	2.39	0.54
1:G:167:TRP:CZ2	3:I:1:LYS:HE3	2.43	0.53
1:A:17:LEU:CG	1:A:18:GLU:H	2.21	0.53
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.43	0.53
1:J:82:LEU:HA	1:J:87:GLN:HE21	1.73	0.52
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.45	0.52
1:D:261:VAL:HB	1:D:270:LEU:HB2	1.92	0.52
1:J:194:ARG:HG3	1:J:199:VAL:HG12	1.92	0.51
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.45	0.51
2:B:39:MET:HE1	2:B:67:HIS:CA	2.39	0.51
2:E:40:LEU:HD23	2:E:45:LYS:HA	1.93	0.51
1:D:54:GLN:HE22	1:D:174:ASN:HB3	1.77	0.50
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.47	0.50
1:A:144:ARG:HD3	1:A:148:GLU:OE2	2.12	0.49
1:A:32:GLU:OE2	1:A:48:ARG:HD2	2.13	0.49
2:K:79:ALA:HB2	2:K:94:TYR:CD1	2.48	0.49
2:B:59:ASP:O	2:B:60:TRP:HB2	2.13	0.48
1:J:75:ARG:HD2	4:J:283:HOH:O	2.13	0.48
1:D:202:ARG:HD2	1:D:244:TRP:CE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:50:GLU:HB2	2:E:67:HIS:CE1	2.49	0.48
1:G:234:ARG:HD3	2:H:10:TYR:CZ	2.48	0.48
1:J:6:ARG:NH2	1:J:113:TYR:CE2	2.82	0.48
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.49	0.47
1:J:266:LEU:HD21	1:J:270:LEU:HG	1.96	0.47
1:G:260:ARG:HA	1:G:270:LEU:O	2.15	0.47
1:G:72:GLN:HE22	1:G:75:ARG:NH1	2.13	0.47
2:H:1:ILE:O	2:H:1:ILE:CG2	2.59	0.47
2:K:39:MET:HE1	2:K:67:HIS:C	2.35	0.46
1:A:11:ALA:HA	1:A:21:ARG:O	2.15	0.46
1:G:230:LEU:O	1:G:230:LEU:HD12	2.16	0.46
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.50	0.46
1:G:118:TYR:CD2	1:G:119:GLU:HG2	2.51	0.45
1:J:263:HIS:ND1	1:J:264:GLU:O	2.46	0.45
2:H:39:MET:HE3	2:H:49:VAL:HG13	1.97	0.45
1:G:47:PRO:HG3	1:G:60:TRP:CZ2	2.51	0.45
1:D:108:ARG:NE	1:J:214:THR:HG21	2.31	0.45
1:G:66:LYS:HD2	3:I:2:ALA:HB3	1.99	0.45
1:A:219:LEU:HB2	1:A:224:LEU:HD11	1.98	0.44
1:G:228:MET:CE	1:G:245:ALA:HB1	2.47	0.44
1:A:82:LEU:HA	1:A:87:GLN:HE21	1.83	0.44
1:A:255:GLN:HE22	1:A:274:TRP:HB3	1.83	0.44
1:D:220:ASN:O	1:D:220:ASN:OD1	2.36	0.44
1:J:219:LEU:C	1:J:220:ASN:HD22	2.22	0.43
1:J:255:GLN:HE22	1:J:274:TRP:C	2.22	0.43
2:K:39:MET:HE3	2:K:49:VAL:HG13	2.00	0.43
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.54	0.42
1:J:234:ARG:HD3	2:K:10:TYR:CZ	2.53	0.42
1:J:111:ARG:HD2	1:J:113:TYR:OH	2.18	0.42
1:A:230:LEU:C	1:A:230:LEU:HD12	2.39	0.42
1:D:82:LEU:HA	1:D:87:GLN:HE21	1.85	0.42
2:H:39:MET:HE1	2:H:67:HIS:C	2.40	0.42
2:H:39:MET:CE	2:H:49:VAL:HG13	2.49	0.42
1:J:77:SER:HB3	3:L:9:ILE:HB	2.02	0.42
1:J:35:ARG:NH2	2:K:54:MET:O	2.51	0.42
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.55	0.42
1:D:11:ALA:HA	1:D:21:ARG:O	2.19	0.41
1:D:176:ASN:O	1:D:180:LEU:HB2	2.20	0.41
1:J:142:ILE:HD13	1:J:142:ILE:N	2.35	0.41
1:J:228:MET:CE	1:J:245:ALA:HB1	2.51	0.41
2:E:39:MET:HE1	2:E:68:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:VAL:HG23	1:G:33:PHE:CE1	2.56	0.41
1:G:32:GLU:OE2	1:G:35:ARG:HD2	2.22	0.40
1:J:219:LEU:HD13	1:J:257:TYR:CZ	2.57	0.40
1:G:193:PRO:O	1:G:199:VAL:HA	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	271/276 (98%)	259 (96%)	11 (4%)	1 (0%)	34	60
1	D	271/276 (98%)	253 (93%)	15 (6%)	3 (1%)	14	34
1	G	271/276 (98%)	256 (94%)	13 (5%)	2 (1%)	22	46
1	J	271/276 (98%)	258 (95%)	9 (3%)	4 (2%)	10	26
2	B	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
2	E	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	H	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	K	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	I	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1500/1536 (98%)	1425 (95%)	64 (4%)	11 (1%)	22	46

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	193	PRO
1	G	194	ARG
1	A	17	LEU
1	D	265	GLY
3	C	6	TYR
1	D	264	GLU
1	J	193	PRO
1	J	220	ASN
1	D	193	PRO
1	J	197	GLY
1	J	221	GLY

### 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	232/234 (99%)	216 (93%)	16 (7%)	15	35
1	D	232/234 (99%)	216 (93%)	16 (7%)	15	35
1	G	232/234 (99%)	219 (94%)	13 (6%)	21	45
1	J	232/234 (99%)	215 (93%)	17 (7%)	14	33
2	B	94/94 (100%)	84 (89%)	10 (11%)	6	15
2	E	94/94 (100%)	86 (92%)	8 (8%)	10	24
2	H	94/94 (100%)	87 (93%)	7 (7%)	13	32
2	K	94/94 (100%)	86 (92%)	8 (8%)	10	24
3	C	7/7 (100%)	6 (86%)	1 (14%)	3	8
3	F	7/7 (100%)	7 (100%)	0	100	100
3	I	7/7 (100%)	7 (100%)	0	100	100
3	L	7/7 (100%)	7 (100%)	0	100	100
All	All	1332/1340 (99%)	1236 (93%)	96 (7%)	14	34

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	31	LYS
1	A	38	SER
1	A	48	ARG
1	A	78	LEU
1	A	82	LEU
1	A	99	SER
1	A	111	ARG
1	A	114	LEU
1	A	121	ARG
1	A	178	THR
1	A	220	ASN
1	A	222	GLU
1	A	229	GLU
1	A	234	ARG
1	A	270	LEU
2	B	1	ILE
2	B	4	THR
2	B	39	MET
2	B	48	LYS
2	B	54	MET
2	B	64	ILE
2	B	70	PHE
2	B	75	THR
2	B	83	LYS
2	B	93	VAL
3	C	1	LYS
1	D	17	LEU
1	D	31	LYS
1	D	39	ASP
1	D	45	TYR
1	D	48	ARG
1	D	53	GLU
1	D	78	LEU
1	D	82	LEU
1	D	111	ARG
1	D	114	LEU
1	D	194	ARG
1	D	215	LEU
1	D	220	ASN
1	D	222	GLU
1	D	234	ARG
1	D	255	GLN

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Mol	Chain	Res	Type
2	E	1	ILE
2	E	2	GLN
2	E	4	THR
2	E	54	MET
2	E	58	LYS
2	E	70	PHE
2	E	75	THR
2	E	93	VAL
1	G	35	ARG
1	G	44	ARG
1	G	48	ARG
1	G	53	GLU
1	G	78	LEU
1	G	82	LEU
1	G	111	ARG
1	G	176	ASN
1	G	178	THR
1	G	194	ARG
1	G	225	THR
1	G	234	ARG
1	G	248	VAL
2	H	1	ILE
2	H	4	THR
2	H	54	MET
2	H	70	PHE
2	H	75	THR
2	H	93	VAL
2	H	98	ASP
1	J	18	GLU
1	J	44	ARG
1	J	48	ARG
1	J	75	ARG
1	J	78	LEU
1	J	82	LEU
1	J	111	ARG
1	J	115	GLN
1	J	176	ASN
1	J	181	ARG
1	J	186	LYS
1	J	194	ARG
1	J	220	ASN
1	J	225	THR

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Mol	Chain	Res	Type
1	J	230	LEU
1	J	234	ARG
1	J	248	VAL
2	K	1	ILE
2	K	4	THR
2	K	29	GLN
2	K	58	LYS
2	K	70	PHE
2	K	74	GLU
2	K	75	THR
2	K	93	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	87	GLN
1	A	97	GLN
1	A	255	GLN
3	C	5	ASN
1	D	54	GLN
1	D	87	GLN
1	D	97	GLN
1	D	226	GLN
3	F	5	ASN
1	G	72	GLN
1	G	87	GLN
1	G	97	GLN
1	G	192	HIS
1	G	220	ASN
1	G	226	GLN
3	I	5	ASN
1	J	87	GLN
1	J	97	GLN
1	J	155	HIS
1	J	192	HIS
1	J	220	ASN
1	J	255	GLN
2	K	67	HIS
3	L	5	ASN

### 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 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 ⓘ

### 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	273/276 (98%)	0.27	14 (5%) 28 26	28, 45, 84, 89	0
1	D	273/276 (98%)	0.62	36 (13%) 3 2	28, 45, 84, 90	0
1	G	273/276 (98%)	0.54	35 (12%) 3 3	28, 45, 84, 90	0
1	J	273/276 (98%)	0.43	30 (10%) 5 4	30, 45, 84, 91	0
2	B	99/99 (100%)	-0.08	0 100 100	34, 45, 54, 59	0
2	E	99/99 (100%)	0.09	2 (2%) 65 67	34, 45, 54, 60	0
2	H	99/99 (100%)	0.15	3 (3%) 50 51	33, 45, 54, 63	0
2	K	99/99 (100%)	-0.04	1 (1%) 82 83	34, 45, 55, 60	0
3	C	9/9 (100%)	0.27	0 100 100	33, 35, 39, 39	0
3	F	9/9 (100%)	0.30	0 100 100	33, 36, 39, 40	0
3	I	9/9 (100%)	0.25	0 100 100	33, 35, 39, 39	0
3	L	9/9 (100%)	0.79	0 100 100	33, 36, 40, 40	0
All	All	1524/1536 (99%)	0.35	121 (7%) 12 10	28, 45, 83, 91	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	178	THR	10.8
1	D	177	ALA	9.3
1	D	194	ARG	8.6
1	D	178	THR	8.3
1	G	177	ALA	7.8
1	G	196	LYS	7.3
2	H	99	MET	7.1
1	A	177	ALA	6.7
1	J	178	THR	6.3
1	J	194	ARG	6.1
1	A	178	THR	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	196	LYS	6.0
1	G	249	VAL	6.0
1	J	179	LEU	6.0
1	G	179	LEU	5.9
1	G	251	LEU	5.8
1	J	197	GLY	5.8
1	D	249	VAL	5.6
1	D	220	ASN	5.5
1	G	197	GLY	5.5
1	A	179	LEU	5.2
1	J	225	THR	5.1
1	J	177	ALA	5.1
1	D	179	LEU	4.8
1	D	252	GLY	4.7
1	G	195	SER	4.6
1	G	221	GLY	4.5
1	J	193	PRO	4.5
1	J	251	LEU	4.4
1	D	16	GLY	4.3
1	G	198	GLU	4.3
1	D	17	LEU	4.2
1	D	181	ARG	4.1
1	A	176	ASN	4.1
1	J	220	ASN	4.0
1	A	16	GLY	4.0
1	D	248	VAL	4.0
1	G	252	GLY	4.0
1	G	220	ASN	3.9
1	G	248	VAL	3.8
1	D	15	PRO	3.7
1	D	193	PRO	3.7
2	E	47	PRO	3.6
1	G	194	ARG	3.6
1	A	18	GLU	3.4
1	J	224	LEU	3.4
1	J	226	GLN	3.4
1	J	250	PRO	3.3
1	J	252	GLY	3.3
1	G	191	HIS	3.3
1	J	58	GLU	3.3
1	D	197	GLY	3.2
1	G	226	GLN	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	J	196	LYS	3.2
1	G	273	ARG	3.2
1	D	195	SER	3.2
1	D	256	ASN	3.1
1	A	99	SER	3.1
1	J	57	PRO	3.1
2	K	44	LYS	3.0
1	D	18	GLU	3.0
1	G	255	GLN	3.0
1	D	180	LEU	3.0
1	J	180	LEU	2.9
1	D	199	VAL	2.9
1	D	41	GLU	2.9
1	G	270	LEU	2.8
1	A	44	ARG	2.8
1	G	200	THR	2.8
1	G	193	PRO	2.8
2	E	16	GLU	2.7
1	G	227	ASP	2.7
1	J	222	GLU	2.7
1	D	201	LEU	2.7
1	D	42	ASN	2.7
1	D	227	ASP	2.7
1	G	190	THR	2.6
1	J	176	ASN	2.6
1	G	176	ASN	2.5
1	A	273	ARG	2.5
1	D	273	ARG	2.5
1	J	62	ARG	2.5
1	G	250	PRO	2.5
1	J	253	LYS	2.5
1	J	248	VAL	2.4
1	G	18	GLU	2.4
1	J	18	GLU	2.4
1	D	192	HIS	2.4
1	A	42	ASN	2.4
1	D	186	LYS	2.4
1	G	254	GLU	2.4
1	A	220	ASN	2.3
1	A	181	ARG	2.3
1	A	41	GLU	2.3
1	J	195	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	41	GLU	2.3
1	G	257	TYR	2.3
1	G	16	GLY	2.3
1	G	222	GLU	2.2
1	D	253	LYS	2.2
2	H	48	LYS	2.2
1	J	249	VAL	2.2
1	D	191	HIS	2.2
1	J	227	ASP	2.2
1	J	221	GLY	2.2
1	G	256	ASN	2.2
1	D	219	LEU	2.2
1	J	239	GLY	2.2
1	G	199	VAL	2.2
1	G	225	THR	2.1
1	G	192	HIS	2.1
1	D	251	LEU	2.1
1	J	89	ALA	2.1
1	A	79	ARG	2.1
1	G	253	LYS	2.1
1	D	198	GLU	2.1
1	D	221	GLY	2.0
1	D	10	THR	2.0
1	D	274	TRP	2.0
2	H	47	PRO	2.0
1	D	229	GLU	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.