



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 25, 2024 – 10:05 AM EST

PDB ID : 8EB2
Title : Structure of HLA-A*02:01 in complex with NY-ESO-1 peptide and PA2.1 Fab
Authors : Jette, C.A.; West, A.P.
Deposited on : 2022-08-30
Resolution : 2.90 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

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>.

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 : 2.36
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) : 2.36

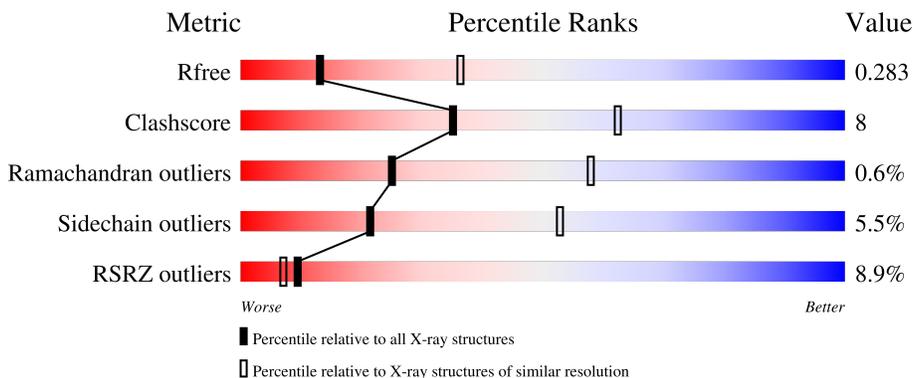
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 ≥ 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	 77% 21%
1	D	275	 77% 23%
1	G	275	 79% 20%
2	B	100	 84% 16%
2	E	100	 7% 87% 13%

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Mol	Chain	Length	Quality of chain
2	H	100	<p>5% 85% 13%</p>
3	C	9	<p>56% 44%</p>
3	F	9	<p>33% 56% 11%</p>
3	I	9	<p>11% 67% 22% 11%</p>
4	J	221	<p>2% 71% 22%</p>
4	K	221	<p>23% 75% 21%</p>
4	N	221	<p>38% 62% 31% 5%</p>
5	L	219	<p>78% 21%</p>
5	M	219	<p>5% 81% 16%</p>
5	O	219	<p>22% 78% 19%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19374 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-A*02:01 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	Total 2246	C 1403	N 409	O 425	S 9	0	0	0
1	D	274	Total 2237	C 1398	N 408	O 422	S 9	0	0	0
1	G	275	Total 2246	C 1403	N 409	O 425	S 9	0	0	0

- 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 837	C 533	N 141	O 159	S 4	0	0	0
2	E	100	Total 836	C 533	N 141	O 158	S 4	0	0	0
2	H	100	Total 836	C 533	N 141	O 158	S 4	0	0	0

There are 3 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
H	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called NY-ESO-1 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	9	Total 75	C 51	N 11	O 12	S 1	0	0	0
3	F	9	Total 75	C 51	N 11	O 12	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	9	75	51	11	12	1	0	0	0

- Molecule 4 is a protein called PA2.1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	J	215	1628	1032	267	323	6	0	0	0
4	K	215	1628	1032	267	323	6	0	0	0
4	N	215	1628	1032	267	323	6	0	0	0

- Molecule 5 is a protein called PA2.1 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	L	218	1683	1052	288	338	5	0	0	0
5	M	217	1671	1044	287	335	5	0	0	0
5	O	217	1673	1046	287	335	5	0	0	0

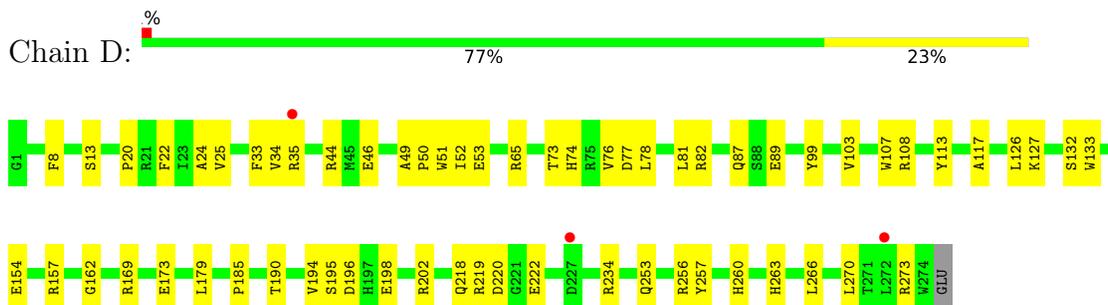
3 Residue-property plots [i](#)

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

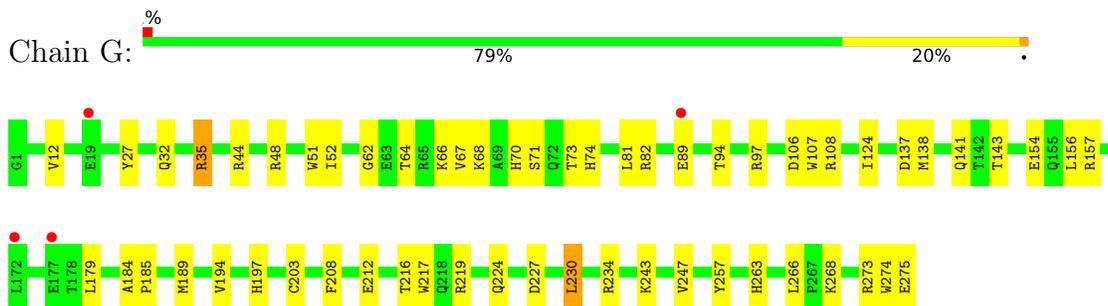
- Molecule 1: HLA-A*02:01 alpha chain



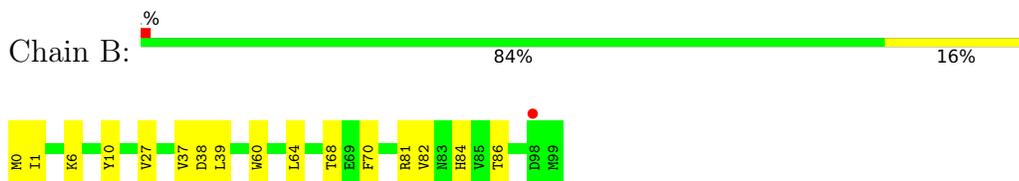
- Molecule 1: HLA-A*02:01 alpha chain



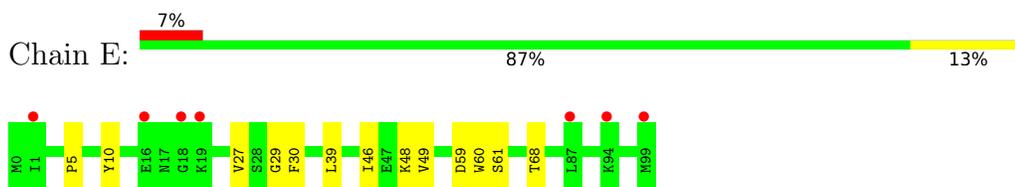
- Molecule 1: HLA-A*02:01 alpha chain



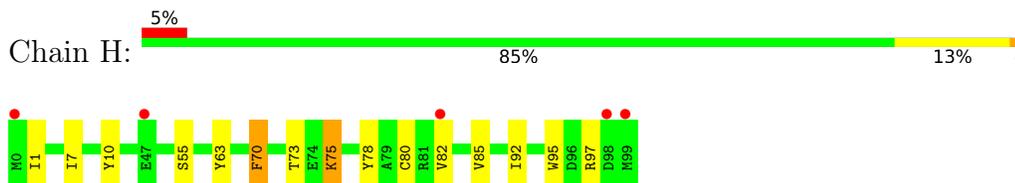
- Molecule 2: Beta-2-microglobulin



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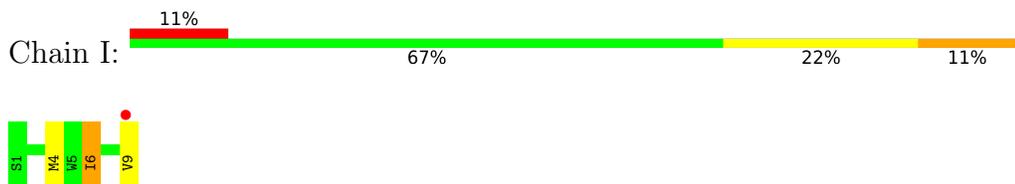
- Molecule 3: NY-ESO-1 peptide



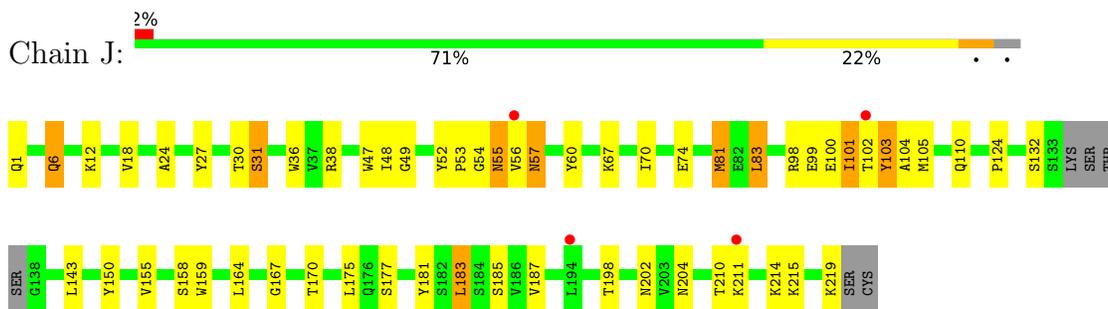
- Molecule 3: NY-ESO-1 peptide



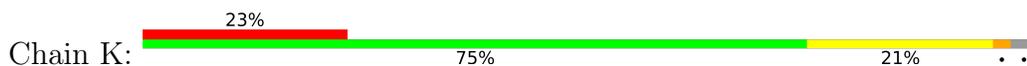
- Molecule 3: NY-ESO-1 peptide

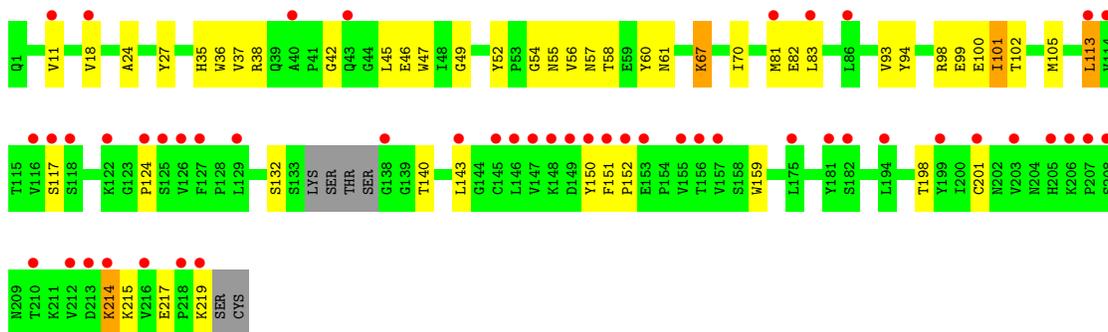


- Molecule 4: PA2.1 Fab Heavy Chain

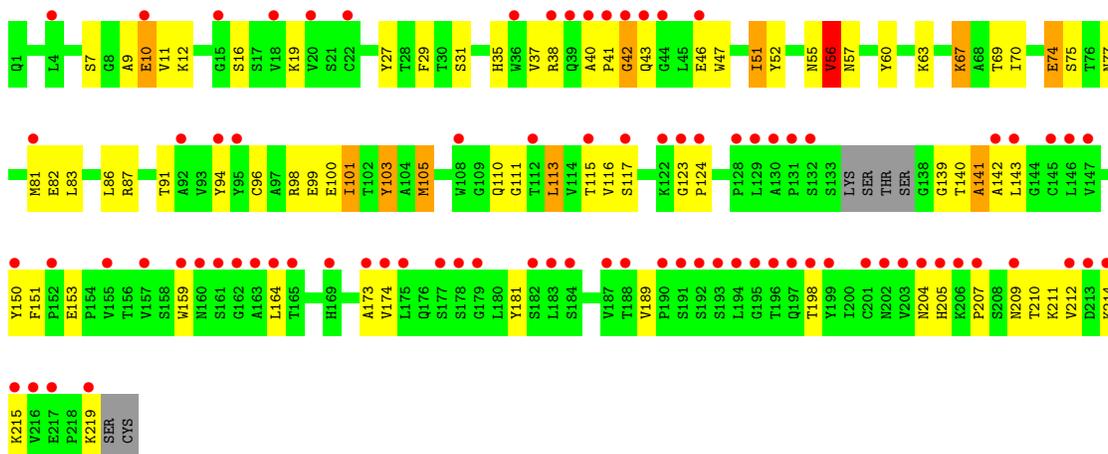


- Molecule 4: PA2.1 Fab Heavy Chain

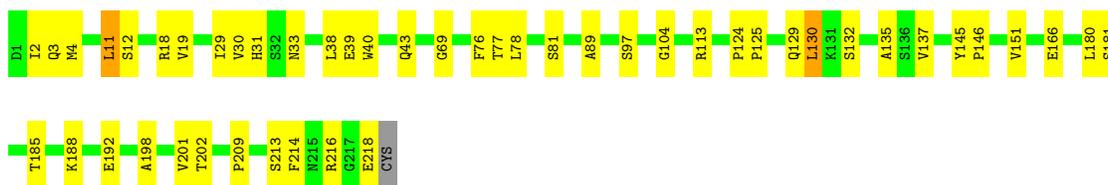




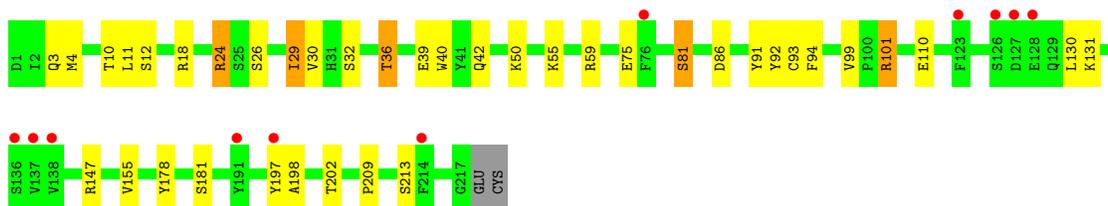
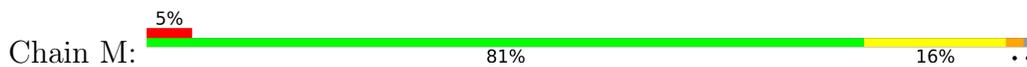
● Molecule 4: PA2.1 Fab Heavy Chain



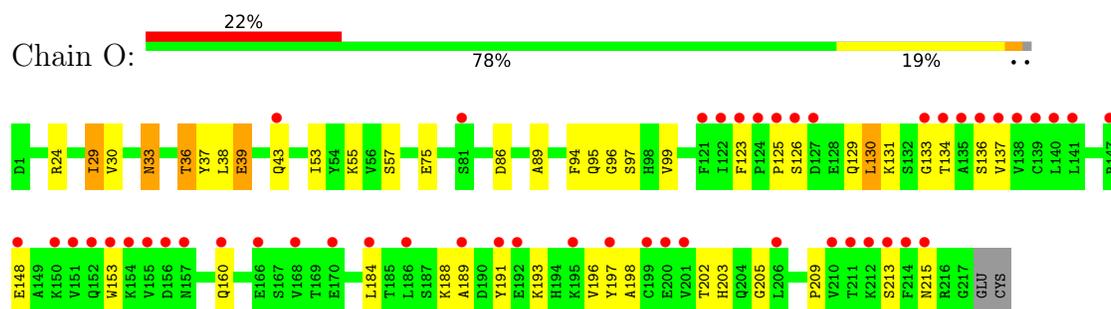
● Molecule 5: PA2.1 Fab Light Chain



● Molecule 5: PA2.1 Fab Light Chain



● Molecule 5: PA2.1 Fab Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.80Å 148.79Å 199.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.59 – 2.90 49.59 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.59-2.90) 83.9 (49.59-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.48 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.239 , 0.284 0.236 , 0.283	Depositor DCC
R_{free} test set	1999 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtrriage
Anisotropy	0.494	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19374	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.54	0/2311	0.74	1/3137 (0.0%)
1	D	0.51	0/2302	0.70	1/3125 (0.0%)
1	G	0.48	0/2311	0.70	1/3137 (0.0%)
2	B	0.56	0/860	0.74	1/1162 (0.1%)
2	E	0.45	0/859	0.66	0/1162
2	H	0.43	0/859	0.67	0/1162
3	C	0.38	0/76	0.77	0/103
3	F	0.55	0/76	0.97	0/103
3	I	0.68	0/76	0.83	0/103
4	J	0.53	0/1669	0.71	0/2276
4	K	0.43	0/1669	0.65	0/2276
4	N	0.45	0/1669	0.66	0/2276
5	L	0.59	0/1720	0.78	2/2333 (0.1%)
5	M	0.47	0/1708	0.67	1/2317 (0.0%)
5	O	0.41	0/1710	0.68	0/2319
All	All	0.49	0/19875	0.70	7/26991 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	11	LEU	CB-CG-CD1	-6.24	100.40	111.00
2	B	64	LEU	CB-CG-CD1	-6.00	100.81	111.00
5	L	11	LEU	CA-CB-CG	5.50	127.95	115.30
1	G	156	LEU	CA-CB-CG	5.48	127.91	115.30
5	M	11	LEU	CA-CB-CG	5.14	127.11	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2246	0	2096	46	0
1	D	2237	0	2090	46	0
1	G	2246	0	2096	37	0
2	B	837	0	803	8	0
2	E	836	0	803	11	0
2	H	836	0	803	8	0
3	C	75	0	83	3	0
3	F	75	0	83	7	0
3	I	75	0	83	6	0
4	J	1628	0	1585	38	0
4	K	1628	0	1585	32	0
4	N	1628	0	1585	44	0
5	L	1683	0	1637	24	0
5	M	1671	0	1622	16	0
5	O	1673	0	1627	24	0
All	All	19374	0	18581	312	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 8.

The worst 5 of 312 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:G:70:HIS:HA	3:I:6:ILE:HD11	1.50	0.94
1:A:35:ARG:HD2	1:A:48:ARG:HE	1.35	0.91
1:G:154:GLU:HG3	1:G:157:ARG:HH22	1.36	0.90
1:A:108:ARG:NH1	4:K:99:GLU:OE2	2.11	0.84
4:K:100:GLU:O	4:K:102:THR:N	2.11	0.84

There are no symmetry-related clashes.

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%)	264 (97%)	9 (3%)	0	100	100
1	D	272/275 (99%)	261 (96%)	11 (4%)	0	100	100
1	G	273/275 (99%)	260 (95%)	13 (5%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	E	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
2	H	98/100 (98%)	93 (95%)	5 (5%)	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
3	I	7/9 (78%)	7 (100%)	0	0	100	100
4	J	211/221 (96%)	197 (93%)	12 (6%)	2 (1%)	17	48
4	K	211/221 (96%)	193 (92%)	14 (7%)	4 (2%)	8	28
4	N	211/221 (96%)	192 (91%)	11 (5%)	8 (4%)	3	13
5	L	216/219 (99%)	208 (96%)	8 (4%)	0	100	100
5	M	215/219 (98%)	204 (95%)	11 (5%)	0	100	100
5	O	215/219 (98%)	204 (95%)	10 (5%)	1 (0%)	29	61
All	All	2412/2472 (98%)	2284 (95%)	113 (5%)	15 (1%)	25	58

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	55	ASN
4	J	56	VAL
4	K	101	ILE
4	N	56	VAL
4	N	103	TYR

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%)	223 (96%)	8 (4%)	36	70
1	D	230/231 (100%)	226 (98%)	4 (2%)	60	86
1	G	231/231 (100%)	222 (96%)	9 (4%)	32	66
2	B	95/95 (100%)	94 (99%)	1 (1%)	73	92
2	E	95/95 (100%)	95 (100%)	0	100	100
2	H	95/95 (100%)	91 (96%)	4 (4%)	30	63
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	19
3	F	9/9 (100%)	7 (78%)	2 (22%)	1	3
3	I	9/9 (100%)	8 (89%)	1 (11%)	6	19
4	J	182/188 (97%)	165 (91%)	17 (9%)	9	27
4	K	182/188 (97%)	173 (95%)	9 (5%)	25	57
4	N	182/188 (97%)	162 (89%)	20 (11%)	6	19
5	L	193/194 (100%)	183 (95%)	10 (5%)	23	55
5	M	191/194 (98%)	173 (91%)	18 (9%)	8	26
5	O	192/194 (99%)	180 (94%)	12 (6%)	18	46
All	All	2126/2151 (99%)	2010 (94%)	116 (6%)	21	53

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	K	35	HIS
5	O	75	GLU
5	M	36	THR
5	O	39	GLU
4	N	117	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
5	L	35	ASN
4	K	43	GLN
4	N	110	GLN
4	N	77	ASN
4	J	204	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th 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 ²)	Q<0.9
1	A	275/275 (100%)	0.08	0 100 100	46, 64, 87, 123	0
1	D	274/275 (99%)	0.18	3 (1%) 80 80	45, 66, 163, 202	0
1	G	275/275 (100%)	0.37	4 (1%) 73 73	50, 83, 116, 169	0
2	B	100/100 (100%)	0.27	1 (1%) 82 82	42, 58, 92, 125	0
2	E	100/100 (100%)	0.51	7 (7%) 16 12	54, 93, 139, 158	0
2	H	100/100 (100%)	0.46	5 (5%) 28 25	61, 82, 120, 132	0
3	C	9/9 (100%)	0.82	0 100 100	57, 61, 72, 75	0
3	F	9/9 (100%)	0.33	0 100 100	46, 51, 58, 60	0
3	I	9/9 (100%)	1.11	1 (11%) 5 4	73, 88, 97, 100	0
4	J	215/221 (97%)	0.27	4 (1%) 66 65	46, 68, 106, 127	0
4	K	215/221 (97%)	1.07	50 (23%) 0 0	62, 107, 153, 183	0
4	N	215/221 (97%)	2.06	84 (39%) 0 0	80, 167, 239, 299	0
5	L	218/219 (99%)	0.01	0 100 100	42, 55, 82, 110	0
5	M	217/219 (99%)	0.32	11 (5%) 28 24	61, 80, 130, 147	0
5	O	217/219 (99%)	1.20	49 (22%) 0 0	74, 130, 192, 239	0
All	All	2448/2472 (99%)	0.56	219 (8%) 9 7	42, 79, 176, 299	0

The worst 5 of 219 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	N	194	LEU	12.9
4	N	212	VAL	12.4
4	N	155	VAL	11.3
4	N	203	VAL	10.7
4	N	214	LYS	10.1

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.