



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 9, 2024 – 02:28 PM EST

PDB ID : 8V50
Title : Crystal structure of a HLA-B*35:01-NP6 with D1 TCR
Authors : Littler, D.R.; Rossjohn, J.; Gras, S.
Deposited on : 2023-11-30
Resolution : 2.65 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) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

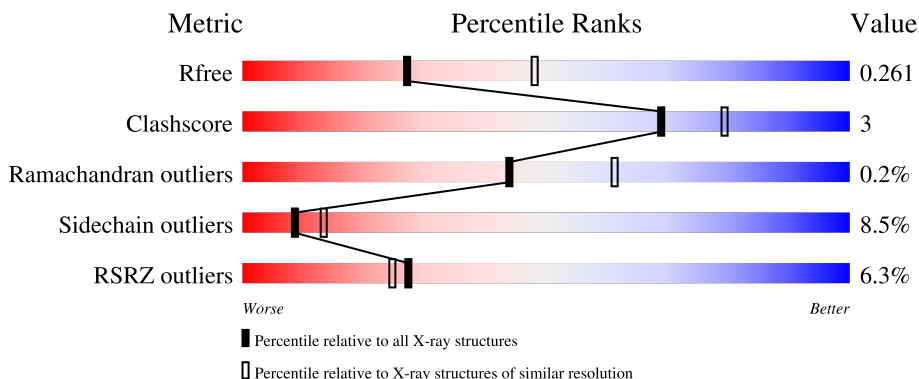
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	164625	1003 (2.66-2.66)
Clashscore	180529	1063 (2.66-2.66)
Ramachandran outliers	177936	1052 (2.66-2.66)
Sidechain outliers	177891	1052 (2.66-2.66)
RSRZ outliers	164620	1003 (2.66-2.66)

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	274	 81% 16% .
1	F	274	 5% 83% 15% .
1	K	274	 4% 80% 19% .
1	P	274	 3% 86% 12% ..
2	B	100	 71% 20% 8% .

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Mol	Chain	Length	Quality of chain
2	G	100	 12% 78% 20%
2	L	100	 8% 75% 22%
2	Q	100	 2% 67% 27% 5%
3	C	9	 78% 22%
3	H	9	 89% 11%
3	M	9	 78% 22%
3	R	9	 89% 11%
4	D	197	 9% 86% 13%
4	I	197	 18% 91% 9%
4	N	197	 11% 91% 8%
4	S	197	 15% 90% 10%
5	E	242	 2% 90% 10%
5	J	242	 6% 88% 12%
5	O	242	 3% 88% 12%
5	T	242	 5% 90% 10%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 27419 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-B35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	Total 2241	C 1397	N 409	O 428	S 7	0	1	0
1	F	273	Total 2241	C 1397	N 409	O 428	S 7	0	1	0
1	K	273	Total 2233	C 1393	N 408	O 425	S 7	0	0	0
1	P	271	Total 2221	C 1386	N 406	O 422	S 7	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	99	Total 829	C 528	N 140	O 158	S 3	0	0	0
2	G	99	Total 829	C 528	N 140	O 158	S 3	0	0	0
2	L	99	Total 829	C 528	N 140	O 158	S 3	0	0	0
2	Q	99	Total 829	C 528	N 140	O 158	S 3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
L	0	MET	-	initiating methionine	UNP P61769
Q	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called NP6 epitope H1N1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			72	47	10	14	1			
3	H	9	Total	C	N	O	S	0	0	0
			72	47	10	14	1			
3	M	9	Total	C	N	O	S	0	0	0
			72	47	10	14	1			
3	R	9	Total	C	N	O	S	0	0	0
			72	47	10	14	1			

- Molecule 4 is a protein called D1 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	0	2	0
			1546	970	249	317	10			
4	I	197	Total	C	N	O	S	0	2	0
			1546	970	249	317	10			
4	N	197	Total	C	N	O	S	0	2	0
			1546	970	249	317	10			
4	S	197	Total	C	N	O	S	0	2	0
			1546	970	249	317	10			

- Molecule 5 is a protein called D1 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	2	0
			1933	1216	338	372	7			
5	J	242	Total	C	N	O	S	0	3	0
			1942	1221	339	375	7			
5	O	242	Total	C	N	O	S	0	3	0
			1942	1221	339	375	7			
5	T	242	Total	C	N	O	S	0	3	0
			1942	1221	339	375	7			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	61	Total	O	0	0
			61	61		
6	B	29	Total	O	0	0
			29	29		
6	C	1	Total	O	0	0
			1	1		

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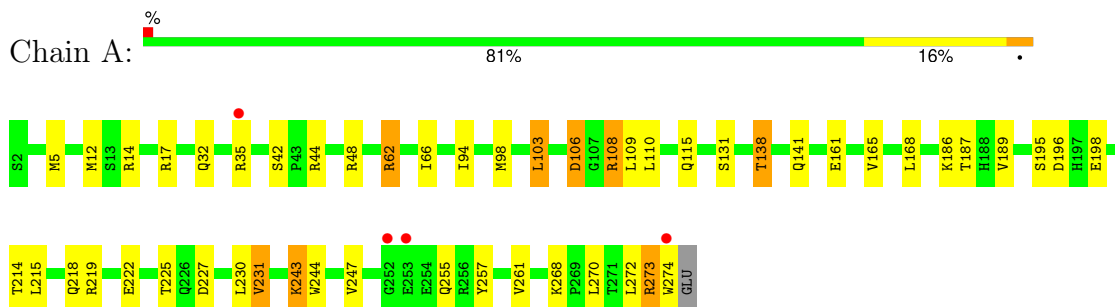
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	44	Total O 44 44	0	0
6	E	50	Total O 50 50	0	0
6	F	83	Total O 83 83	0	0
6	G	22	Total O 22 22	0	0
6	H	6	Total O 6 6	0	0
6	I	65	Total O 65 65	0	0
6	J	73	Total O 73 73	0	0
6	K	86	Total O 86 86	0	0
6	L	14	Total O 14 14	0	0
6	M	5	Total O 5 5	0	0
6	N	58	Total O 58 58	0	0
6	O	73	Total O 73 73	0	0
6	P	89	Total O 89 89	0	0
6	Q	31	Total O 31 31	0	0
6	R	6	Total O 6 6	0	0
6	S	54	Total O 54 54	0	0
6	T	86	Total O 86 86	0	0

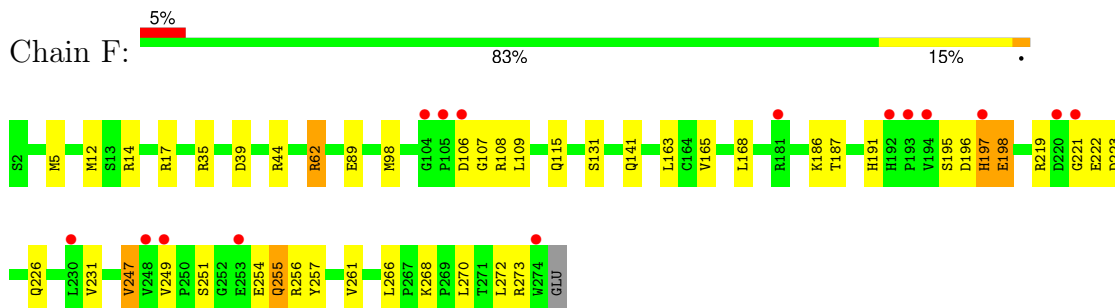
3 Residue-property plots [i](#)

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.

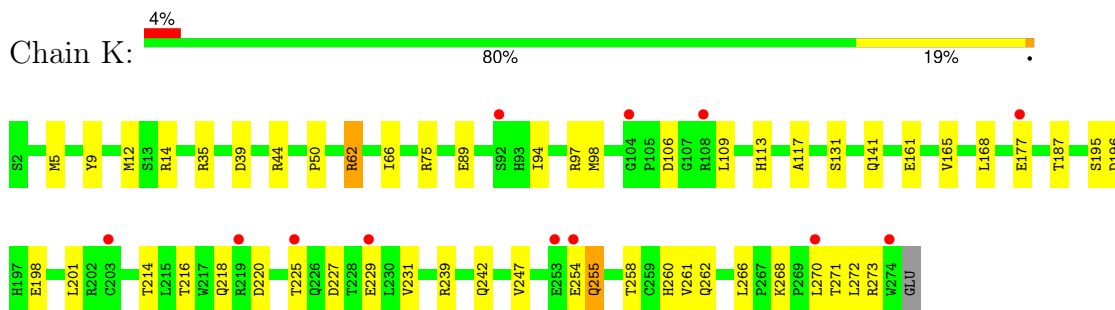
- Molecule 1: HLA-B35



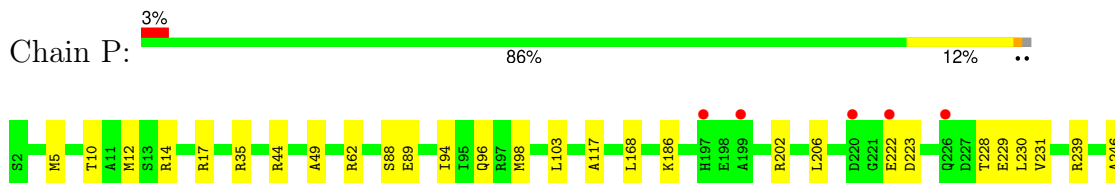
- Molecule 1: HLA-B35

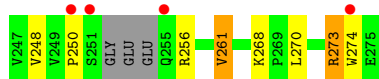


- Molecule 1: HLA-B35

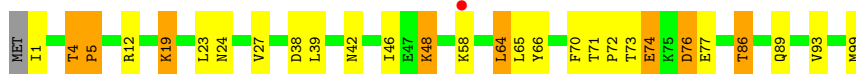


- Molecule 1: HLA-B35

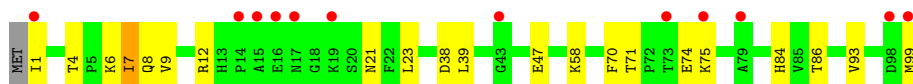
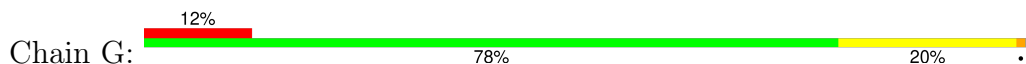




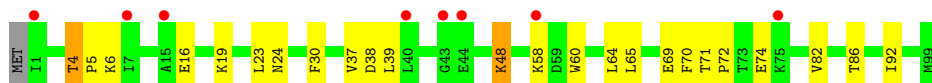
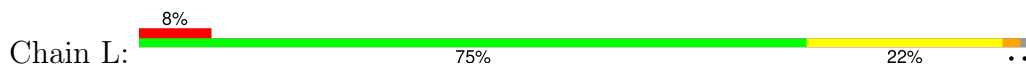
- Molecule 2: Beta-2-microglobulin



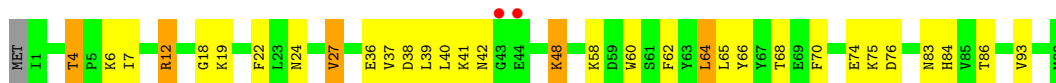
- Molecule 2: Beta-2-microglobulin



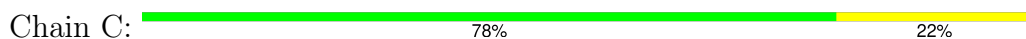
- Molecule 2: Beta-2-microglobulin



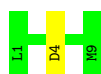
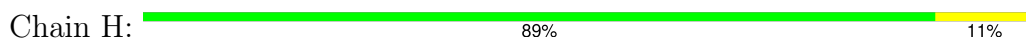
- Molecule 2: Beta-2-microglobulin




- Molecule 3: NP6 epitope H1N1

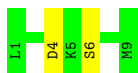


- Molecule 3: NP6 epitope H1N1




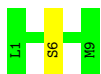
- Molecule 3: NP6 epitope H1N1

Chain M:  78% 22%




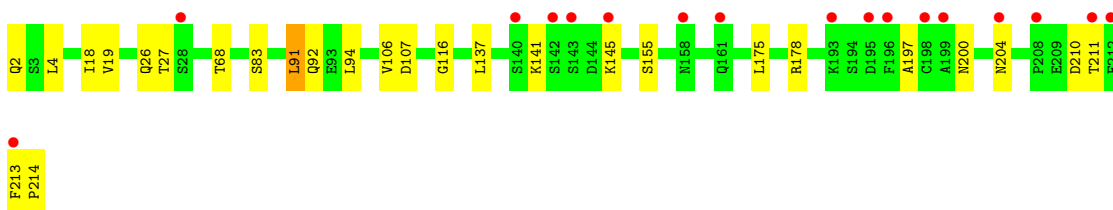
- Molecule 3: NP6 epitope H1N1

Chain R:  89% 11%




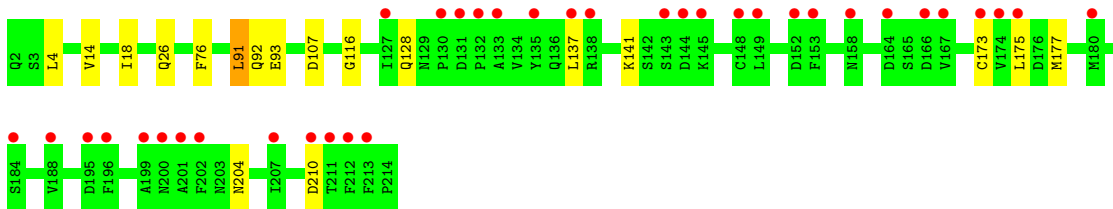
- Molecule 4: D1 TCR alpha chain

Chain D:  9% 86% 13%



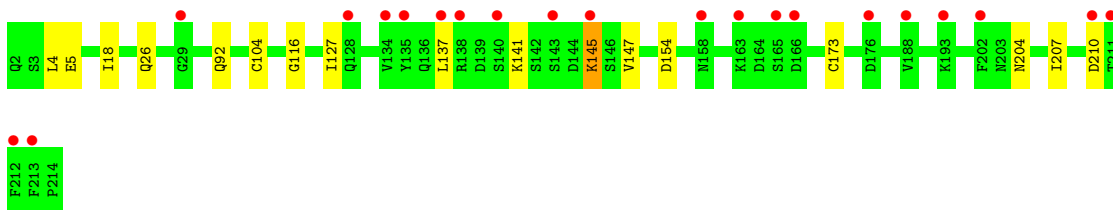
- Molecule 4: D1 TCR alpha chain

Chain I:  18% 91% 9%




- Molecule 4: D1 TCR alpha chain

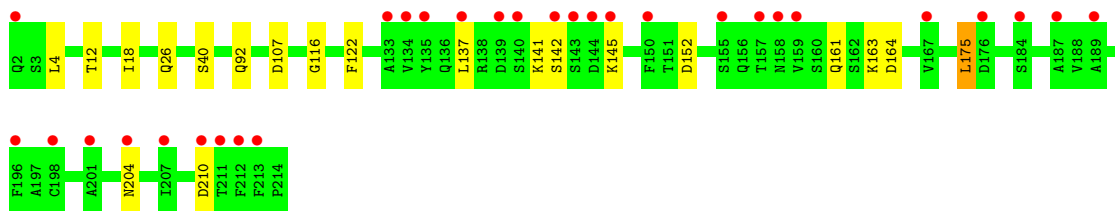
Chain N:  11% 91% 8%



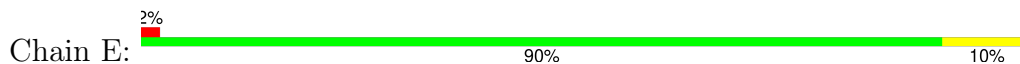
- Molecule 4: D1 TCR alpha chain

Chain S:  15% 90% 10%

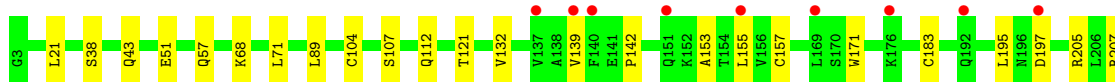
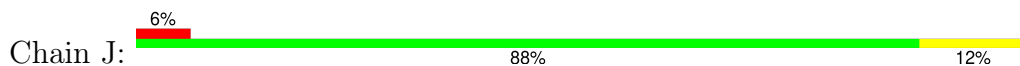




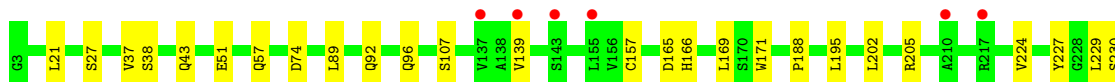
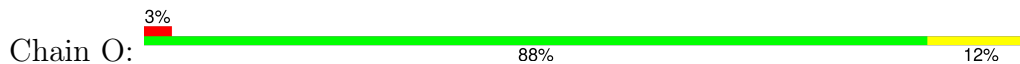
● Molecule 5: D1 TCR beta chain



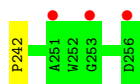
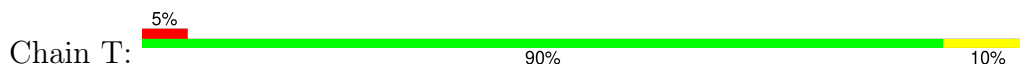
● Molecule 5: D1 TCR beta chain



● Molecule 5: D1 TCR beta chain



● Molecule 5: D1 TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.58Å 192.16Å 252.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.59 – 2.65 38.59 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.59-2.65) 99.9 (38.59-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.218 , 0.265 0.215 , 0.261	Depositor DCC
R_{free} test set	5640 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtrriage
Anisotropy	0.644	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27419	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.27 % 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 4.9819e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.37	0/2303	0.61	0/3132
1	F	0.40	0/2303	0.64	0/3132
1	K	0.39	0/2295	0.62	0/3121
1	P	0.37	0/2282	0.61	0/3101
2	B	0.38	0/852	0.67	0/1152
2	G	0.39	0/852	0.66	0/1152
2	L	0.38	0/852	0.63	0/1152
2	Q	0.38	0/852	0.66	0/1152
3	C	0.57	0/73	0.53	0/96
3	H	0.38	0/73	0.55	0/96
3	M	0.55	0/73	0.58	0/96
3	R	0.39	0/73	0.55	0/96
4	D	0.38	0/1580	0.59	0/2139
4	I	0.37	0/1580	0.59	0/2139
4	N	0.38	0/1580	0.62	0/2139
4	S	0.37	0/1580	0.60	0/2139
5	E	0.36	0/1985	0.58	0/2700
5	J	0.35	0/1994	0.59	0/2712
5	O	0.36	0/1994	0.60	0/2712
5	T	0.35	0/1994	0.60	0/2712
All	All	0.37	0/27170	0.61	0/36870

There are no bond length outliers.

There are no bond angle outliers.

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	2241	0	2101	21	0
1	F	2241	0	2103	16	0
1	K	2233	0	2100	24	0
1	P	2221	0	2090	11	0
2	B	829	0	794	11	0
2	G	829	0	794	5	0
2	L	829	0	794	8	0
2	Q	829	0	794	17	0
3	C	72	0	76	2	0
3	H	72	0	76	1	0
3	M	72	0	76	1	0
3	R	72	0	76	0	0
4	D	1546	0	1437	10	0
4	I	1546	0	1437	9	0
4	N	1546	0	1437	7	0
4	S	1546	0	1437	7	0
5	E	1933	0	1832	9	0
5	J	1942	0	1837	16	0
5	O	1942	0	1837	9	0
5	T	1942	0	1837	13	0
6	A	61	0	0	0	0
6	B	29	0	0	0	0
6	C	1	0	0	0	0
6	D	44	0	0	0	0
6	E	50	0	0	0	0
6	F	83	0	0	0	0
6	G	22	0	0	0	0
6	H	6	0	0	0	0
6	I	65	0	0	0	0
6	J	73	0	0	0	0
6	K	86	0	0	1	0
6	L	14	0	0	0	0
6	M	5	0	0	0	0
6	N	58	0	0	0	0
6	O	73	0	0	0	0
6	P	89	0	0	0	0
6	Q	31	0	0	0	0
6	R	6	0	0	0	0
6	S	54	0	0	0	0
6	T	86	0	0	0	0
All	All	27419	0	24965	173	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 3.

The worst 5 of 173 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)
2:Q:42:ASN:HD21	2:Q:76:ASP:HB2	1.20	1.05
2:Q:42:ASN:HD21	2:Q:76:ASP:CB	1.71	1.03
2:Q:42:ASN:ND2	2:Q:76:ASP:HB2	1.82	0.92
1:A:255:GLN:HG3	1:K:255:GLN:HG2	1.53	0.86
2:G:4:THR:HA	2:G:86:THR:HG21	1.60	0.84

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	272/274 (99%)	266 (98%)	6 (2%)	0	100	100
1	F	272/274 (99%)	262 (96%)	8 (3%)	2 (1%)	19	31
1	K	271/274 (99%)	259 (96%)	12 (4%)	0	100	100
1	P	267/274 (97%)	255 (96%)	10 (4%)	2 (1%)	19	31
2	B	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
2	G	97/100 (97%)	91 (94%)	6 (6%)	0	100	100
2	L	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
2	Q	97/100 (97%)	92 (95%)	4 (4%)	1 (1%)	13	21
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	M	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	197/197 (100%)	187 (95%)	10 (5%)	0	100	100
4	I	197/197 (100%)	185 (94%)	12 (6%)	0	100	100
4	N	197/197 (100%)	182 (92%)	15 (8%)	0	100	100
4	S	197/197 (100%)	183 (93%)	13 (7%)	1 (0%)	25	40
5	E	242/242 (100%)	228 (94%)	14 (6%)	0	100	100
5	J	243/242 (100%)	234 (96%)	9 (4%)	0	100	100
5	O	243/242 (100%)	234 (96%)	8 (3%)	1 (0%)	30	46
5	T	243/242 (100%)	233 (96%)	10 (4%)	0	100	100
All	All	3257/3288 (99%)	3101 (95%)	149 (5%)	7 (0%)	44	61

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	274	TRP
1	P	250	PRO
2	Q	18	GLY
4	S	142	SER
5	O	165	ASP

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	233/233 (100%)	205 (88%)	28 (12%)	4	6
1	F	233/233 (100%)	207 (89%)	26 (11%)	5	8
1	K	232/233 (100%)	205 (88%)	27 (12%)	4	6
1	P	231/233 (99%)	212 (92%)	19 (8%)	9	15
2	B	94/95 (99%)	76 (81%)	18 (19%)	1	1
2	G	94/95 (99%)	81 (86%)	13 (14%)	3	4
2	L	94/95 (99%)	82 (87%)	12 (13%)	3	5
2	Q	94/95 (99%)	80 (85%)	14 (15%)	2	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	9/9 (100%)	8 (89%)	1 (11%)	5	8
3	H	9/9 (100%)	9 (100%)	0	100	100
3	M	9/9 (100%)	8 (89%)	1 (11%)	5	8
3	R	9/9 (100%)	8 (89%)	1 (11%)	5	8
4	D	173/171 (101%)	158 (91%)	15 (9%)	8	13
4	I	173/171 (101%)	164 (95%)	9 (5%)	19	33
4	N	173/171 (101%)	165 (95%)	8 (5%)	23	38
4	S	173/171 (101%)	162 (94%)	11 (6%)	14	25
5	E	210/208 (101%)	195 (93%)	15 (7%)	12	20
5	J	211/208 (101%)	201 (95%)	10 (5%)	22	37
5	O	211/208 (101%)	202 (96%)	9 (4%)	25	41
5	T	211/208 (101%)	202 (96%)	9 (4%)	25	41
All	All	2876/2864 (100%)	2630 (91%)	246 (9%)	8	13

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	99	MET
2	Q	64	LEU
1	K	106	ASP
2	Q	48	LYS
4	S	210	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	Q	42	ASN
5	O	166	HIS
1	K	260	HIS
1	K	113	HIS
5	O	58	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 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, 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	273/274 (99%)	0.13	4 (1%) 71 69	19, 39, 74, 110	2 (0%)
1	F	273/274 (99%)	0.22	15 (5%) 32 29	18, 36, 89, 123	3 (1%)
1	K	273/274 (99%)	0.31	12 (4%) 39 36	20, 38, 90, 114	2 (0%)
1	P	271/274 (98%)	0.05	9 (3%) 49 46	20, 33, 77, 108	1 (0%)
2	B	99/100 (99%)	0.07	1 (1%) 79 77	25, 41, 70, 80	0
2	G	99/100 (99%)	0.67	12 (12%) 10 10	21, 48, 84, 97	0
2	L	99/100 (99%)	0.62	8 (8%) 19 18	23, 54, 95, 104	0
2	Q	99/100 (99%)	0.13	2 (2%) 64 62	21, 38, 76, 84	0
3	C	9/9 (100%)	-0.15	0 100 100	24, 26, 31, 33	0
3	H	9/9 (100%)	-0.24	0 100 100	20, 21, 23, 27	0
3	M	9/9 (100%)	-0.15	0 100 100	22, 23, 26, 29	0
3	R	9/9 (100%)	-0.31	0 100 100	21, 21, 26, 29	0
4	D	197/197 (100%)	0.41	17 (8%) 18 16	11, 39, 117, 136	2 (1%)
4	I	197/197 (100%)	0.71	36 (18%) 4 4	11, 39, 128, 149	2 (1%)
4	N	197/197 (100%)	0.53	21 (10%) 12 12	11, 39, 120, 146	2 (1%)
4	S	197/197 (100%)	0.68	30 (15%) 6 6	11, 40, 129, 157	2 (1%)
5	E	242/242 (100%)	0.11	5 (2%) 63 61	13, 41, 78, 118	2 (0%)
5	J	242/242 (100%)	0.43	14 (5%) 30 28	12, 51, 102, 149	3 (1%)
5	O	242/242 (100%)	0.22	8 (3%) 49 46	12, 45, 88, 134	3 (1%)
5	T	242/242 (100%)	0.23	12 (4%) 35 33	11, 41, 96, 137	3 (1%)
All	All	3278/3288 (99%)	0.32	206 (6%) 27 25	11, 40, 105, 157	27 (0%)

The worst 5 of 206 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	S	211	THR	4.2
5	E	143	SER	4.0
1	K	254	GLU	4.0
1	F	274	TRP	3.8
4	I	211	THR	3.8

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.