



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:48 PM UTC

PDB ID : 6RPB / pdb_00006rpb
Title : Crystal structure of the T-cell receptor NYE_S1 bound to HLA A2*01-SLLMWITQV
Authors : Coles, C.H.; Mulvaney, R.; Malla, S.; Lloyd, A.; Smith, K.; Chester, F.; Knox, A.; Stacey, A.R.; Dukes, J.; Baston, E.; Griffin, S.; Vuidepot, A.; Jakobsen, B.K.; Harper, S.
Deposited on : 2019-05-14
Resolution : 2.50 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

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	:	4-5-2 with Phenix2.0
Xtriage (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

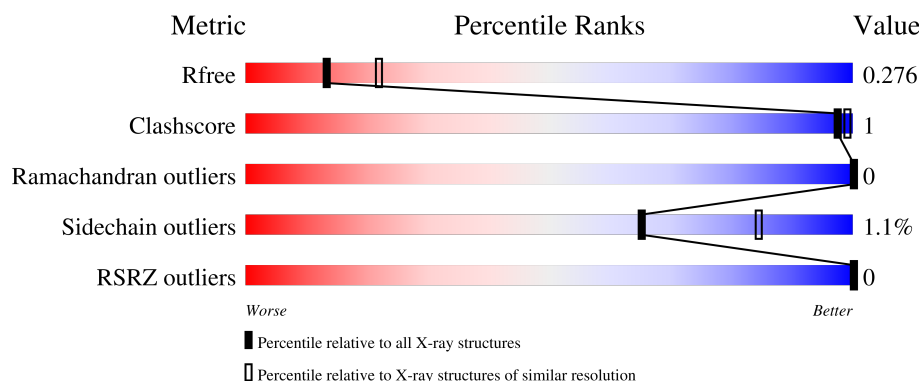
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

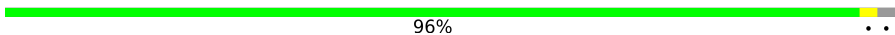
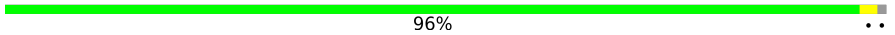
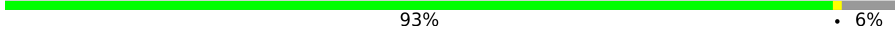
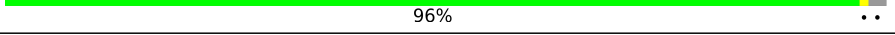
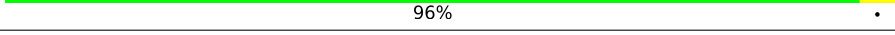
The reported resolution of this entry is 2.50 Å.

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.



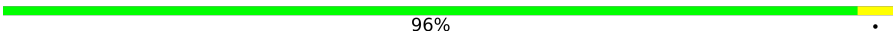
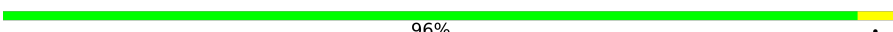
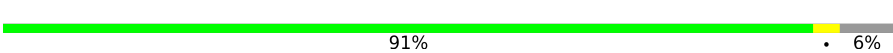
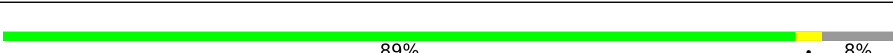
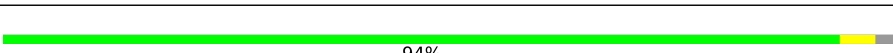
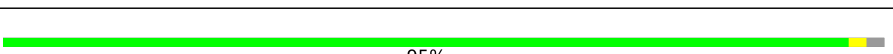
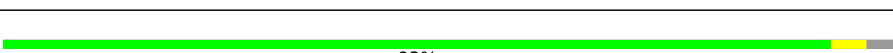
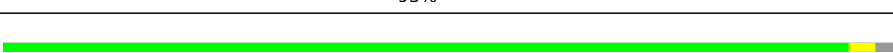
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	277	 96%
1	F	277	 96%
1	K	277	 93% 6%
1	P	277	 96%
2	B	100	 96%

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Mol	Chain	Length	Quality of chain
2	G	100	 96% .
2	L	100	 99% .
2	Q	100	 96% .
3	C	9	 78% 22%
3	H	9	 89% 11%
3	M	9	 89% 11%
3	R	9	 78% 22%
4	D	206	 91% . 6%
4	I	206	 90% . 6%
4	N	206	 87% . 9%
4	S	206	 89% . 8%
5	E	244	 94% . .
5	J	244	 95% . .
5	O	244	 93% . .
5	T	244	 95% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26194 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	271	Total	C	N	O	S	0	0	0
			2216	1388	404	415	9			
1	F	274	Total	C	N	O	S	0	0	0
			2238	1400	405	424	9			
1	K	259	Total	C	N	O	S	0	0	0
			2124	1336	388	391	9			
1	P	271	Total	C	N	O	S	0	0	0
			2213	1385	403	416	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01892
F	0	MET	-	initiating methionine	UNP P01892
K	0	MET	-	initiating methionine	UNP P01892
P	0	MET	-	initiating methionine	UNP P01892

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

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

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 Heteroclitic NY-ESO-1 157-165 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			76	51	11	13	1			
3	H	9	Total	C	N	O	S	0	0	0
			76	51	11	13	1			
3	M	9	Total	C	N	O	S	0	0	0
			76	51	11	13	1			
3	R	9	Total	C	N	O	S	0	0	0
			76	51	11	13	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	194	Total	C	N	O	S	0	0	0
			1512	949	247	308	8			
4	I	194	Total	C	N	O	S	0	0	0
			1515	951	250	306	8			
4	N	188	Total	C	N	O	S	0	0	0
			1465	922	237	298	8			
4	S	189	Total	C	N	O	S	0	0	0
			1476	928	241	299	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	239	Total	C	N	O	S	0	0	0
			1891	1190	328	364	9			
5	J	239	Total	C	N	O	S	0	0	0
			1891	1190	328	364	9			
5	O	237	Total	C	N	O	S	0	0	0
			1876	1182	323	362	9			
5	T	240	Total	C	N	O	S	0	0	0
			1896	1193	329	365	9			

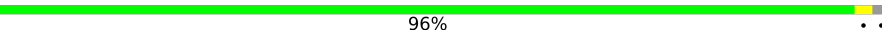
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	21	Total O 21 21	0	0
6	B	9	Total O 9 9	0	0
6	C	5	Total O 5 5	0	0
6	D	15	Total O 15 15	0	0
6	E	15	Total O 15 15	0	0
6	F	19	Total O 19 19	0	0
6	G	12	Total O 12 12	0	0
6	H	4	Total O 4 4	0	0
6	I	10	Total O 10 10	0	0
6	J	16	Total O 16 16	0	0
6	K	14	Total O 14 14	0	0
6	L	5	Total O 5 5	0	0
6	M	4	Total O 4 4	0	0
6	N	10	Total O 10 10	0	0
6	O	14	Total O 14 14	0	0
6	P	14	Total O 14 14	0	0
6	Q	10	Total O 10 10	0	0
6	R	4	Total O 4 4	0	0
6	S	13	Total O 13 13	0	0
6	T	15	Total O 15 15	0	0

3 Residue-property plots [i](#)

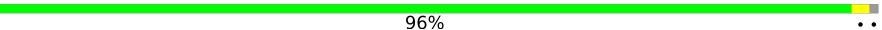
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 class I histocompatibility antigen, A-2 alpha chain

Chain A:  96% ..

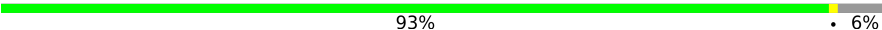


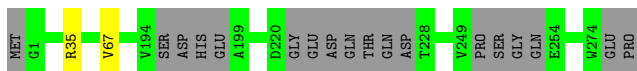
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain F:  96% ..

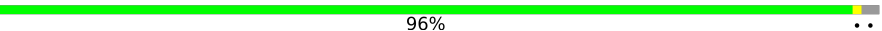


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain K:  93% • 6%

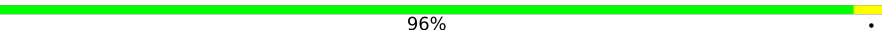


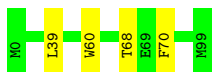
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain P:  96% ..

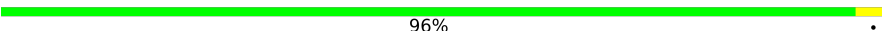


- Molecule 2: Beta-2-microglobulin

Chain B:  96% .

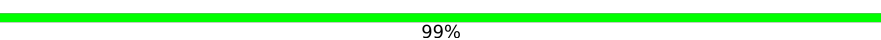


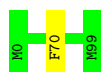
- Molecule 2: Beta-2-microglobulin

Chain G:  96% .

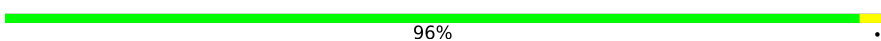


- Molecule 2: Beta-2-microglobulin

Chain L:  99%



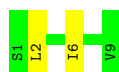
- Molecule 2: Beta-2-microglobulin

Chain Q:  96%



- Molecule 3: Heteroclitic NY-ESO-1 157-165 peptide

Chain C:  78%



- Molecule 3: Heteroclitic NY-ESO-1 157-165 peptide

Chain H:  89%



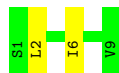
- Molecule 3: Heteroclitic NY-ESO-1 157-165 peptide

Chain M:  89%



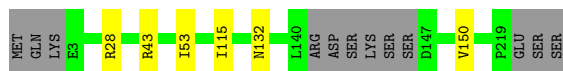
- Molecule 3: Heteroclitic NY-ESO-1 157-165 peptide

Chain R:  78%



- Molecule 4: T-cell receptor alpha chain

Chain D:  91%



- Molecule 4: T-cell receptor alpha chain

Chain I: 90% 6%



- Molecule 4: T-cell receptor alpha chain

Chain N: 87% 9%



- Molecule 4: T-cell receptor alpha chain

Chain S: 89% 8%



- Molecule 5: T-cell receptor beta chain

Chain E: 94%



- Molecule 5: T-cell receptor beta chain

Chain J: 95%



- Molecule 5: T-cell receptor beta chain

Chain O: 93%



- Molecule 5: T-cell receptor beta chain

Chain T: 95%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.34Å 77.13Å 184.63Å 93.02° 93.45° 108.16°	Depositor
Resolution (Å)	73.09 – 2.50 73.09 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (73.09-2.50) 89.8 (73.09-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.249 , 0.273 0.251 , 0.276	Depositor DCC
R_{free} test set	6543 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.766	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 14.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.176 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26194	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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

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	0.54	0/2281	0.76	0/3096
1	F	0.54	0/2303	0.74	1/3127 (0.0%)
1	K	0.51	0/2184	0.74	0/2960
1	P	0.52	0/2277	0.73	0/3089
2	B	0.54	0/860	0.66	0/1162
2	G	0.53	0/860	0.67	0/1162
2	L	0.52	0/860	0.65	0/1162
2	Q	0.52	0/860	0.65	0/1162
3	C	0.49	0/77	0.84	0/103
3	H	0.48	0/77	0.69	0/103
3	M	0.48	0/77	0.57	0/103
3	R	0.50	0/77	0.69	0/103
4	D	0.54	0/1548	0.68	0/2101
4	I	0.55	0/1551	0.68	0/2104
4	N	0.54	0/1499	0.68	0/2034
4	S	0.53	0/1510	0.67	0/2048
5	E	0.54	0/1942	0.68	0/2646
5	J	0.53	0/1942	0.68	0/2646
5	O	0.53	0/1927	0.69	0/2627
5	T	0.52	0/1947	0.67	0/2653
All	All	0.53	0/26659	0.70	1/36191 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	42	SER	N-CA-C	5.16	116.90	111.28

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	2216	0	2074	2	0
1	F	2238	0	2086	5	0
1	K	2124	0	2002	0	0
1	P	2213	0	2068	2	0
2	B	837	0	803	2	0
2	G	837	0	803	3	0
2	L	837	0	803	0	0
2	Q	837	0	803	2	0
3	C	76	0	83	1	0
3	H	76	0	83	1	0
3	M	76	0	83	0	0
3	R	76	0	83	1	0
4	D	1512	0	1414	4	0
4	I	1515	0	1423	4	0
4	N	1465	0	1366	6	0
4	S	1476	0	1379	3	0
5	E	1891	0	1800	7	0
5	J	1891	0	1800	5	0
5	O	1876	0	1784	7	0
5	T	1896	0	1805	5	0
6	A	21	0	0	0	0
6	B	9	0	0	0	0
6	C	5	0	0	0	0
6	D	15	0	0	0	0
6	E	15	0	0	0	0
6	F	19	0	0	0	0
6	G	12	0	0	0	0
6	H	4	0	0	0	0
6	I	10	0	0	0	0
6	J	16	0	0	0	0
6	K	14	0	0	0	0
6	L	5	0	0	0	0
6	M	4	0	0	0	0
6	N	10	0	0	0	0
6	O	14	0	0	0	0
6	P	14	0	0	0	0
6	Q	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	4	0	0	0	0
6	S	13	0	0	0	0
6	T	15	0	0	0	0
All	All	26194	0	24545	38	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 1.

All (38) 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)
4:D:150:VAL:HG11	5:E:158:VAL:HG21	1.73	0.69
4:D:43:ARG:HB2	4:D:53:ILE:HD11	1.78	0.65
4:S:43:ARG:HB2	4:S:53:ILE:HD11	1.79	0.65
4:N:43:ARG:HB2	4:N:53:ILE:HD11	1.80	0.64
4:I:43:ARG:HB2	4:I:53:ILE:HD11	1.79	0.62
4:N:150:VAL:HG11	5:O:158:VAL:HG21	1.82	0.61
4:I:150:VAL:HG11	5:J:158:VAL:HG21	1.82	0.60
4:S:115:ILE:HD11	5:T:55:TYR:CE1	2.38	0.58
4:S:150:VAL:HG11	5:T:158:VAL:HG21	1.86	0.56
4:D:115:ILE:HD11	5:E:55:TYR:CE1	2.41	0.55
5:E:74:ASN:HB3	1:F:42:SER:HA	1.88	0.55
1:P:45:MET:CE	3:R:2:LEU:HD11	2.37	0.54
1:F:45:MET:CE	3:H:2:LEU:HD11	2.40	0.51
4:N:115:ILE:HD11	5:O:55:TYR:CE1	2.48	0.48
4:N:52:LEU:HD22	5:O:115:ALA:CB	2.44	0.47
5:E:141:VAL:HG23	5:E:251:ALA:HB3	1.97	0.47
5:T:141:VAL:HG23	5:T:251:ALA:HB3	1.96	0.47
5:O:141:VAL:HG23	5:O:251:ALA:HB3	1.96	0.46
5:J:141:VAL:HG23	5:J:251:ALA:HB3	1.97	0.46
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.51	0.45
1:P:202:ARG:NH2	2:Q:99:MET:HE2	2.32	0.45
2:G:27:VAL:HG21	2:G:35:ILE:CD1	2.47	0.44
4:N:52:LEU:HD22	5:O:115:ALA:HB3	1.97	0.44
5:T:19:MET:HE2	5:T:21:LEU:HD23	1.99	0.44
5:E:93:SER:OG	1:F:19:GLU:OE2	2.33	0.44
2:G:27:VAL:HG21	2:G:35:ILE:HD11	2.00	0.44
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.53	0.43
4:D:28:ARG:NH2	4:N:131:GLN:O	2.51	0.43
5:E:134:VAL:HG11	5:E:231:LEU:HD13	1.99	0.43
5:O:129:GLU:OE2	2:Q:45:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:LEU:HD23	2:B:68:THR:HG22	2.01	0.42
5:T:134:VAL:HG11	5:T:231:LEU:HD13	2.01	0.42
5:O:134:VAL:HG11	5:O:231:LEU:HD13	2.02	0.42
5:J:134:VAL:HG11	5:J:231:LEU:HD13	2.00	0.41
4:I:178:LEU:HB3	5:J:185:CYS:HB2	2.03	0.41
1:A:45:MET:CE	3:C:2:LEU:HD11	2.51	0.41
4:I:115:ILE:HD11	5:J:55:TYR:CE1	2.55	0.41
5:E:15:THR:HG21	1:F:39:ASP:OD2	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	267/277 (96%)	261 (98%)	6 (2%)	0	100	100
1	F	270/277 (98%)	263 (97%)	7 (3%)	0	100	100
1	K	251/277 (91%)	246 (98%)	5 (2%)	0	100	100
1	P	267/277 (96%)	260 (97%)	7 (3%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	G	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	L	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	Q	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
3	M	7/9 (78%)	7 (100%)	0	0	100	100
3	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	190/206 (92%)	183 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	190/206 (92%)	183 (96%)	7 (4%)	0	100	100
4	N	182/206 (88%)	177 (97%)	5 (3%)	0	100	100
4	S	183/206 (89%)	178 (97%)	5 (3%)	0	100	100
5	E	237/244 (97%)	231 (98%)	6 (2%)	0	100	100
5	J	237/244 (97%)	231 (98%)	6 (2%)	0	100	100
5	O	235/244 (96%)	228 (97%)	7 (3%)	0	100	100
5	T	238/244 (98%)	231 (97%)	7 (3%)	0	100	100
All	All	3167/3344 (95%)	3087 (98%)	80 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	228/233 (98%)	225 (99%)	3 (1%)	61	82
1	F	231/233 (99%)	229 (99%)	2 (1%)	70	87
1	K	217/233 (93%)	215 (99%)	2 (1%)	70	87
1	P	227/233 (97%)	225 (99%)	2 (1%)	70	87
2	B	95/95 (100%)	94 (99%)	1 (1%)	65	84
2	G	95/95 (100%)	94 (99%)	1 (1%)	65	84
2	L	95/95 (100%)	94 (99%)	1 (1%)	65	84
2	Q	95/95 (100%)	93 (98%)	2 (2%)	47	74
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	12
3	H	9/9 (100%)	9 (100%)	0	100	100
3	M	9/9 (100%)	8 (89%)	1 (11%)	6	12
3	R	9/9 (100%)	8 (89%)	1 (11%)	6	12
4	D	172/184 (94%)	171 (99%)	1 (1%)	78	91
4	I	172/184 (94%)	169 (98%)	3 (2%)	53	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	N	166/184 (90%)	163 (98%)	3 (2%)	51	77
4	S	167/184 (91%)	165 (99%)	2 (1%)	63	83
5	E	208/211 (99%)	207 (100%)	1 (0%)	81	92
5	J	208/211 (99%)	207 (100%)	1 (0%)	81	92
5	O	207/211 (98%)	206 (100%)	1 (0%)	81	92
5	T	208/211 (99%)	206 (99%)	2 (1%)	68	86
All	All	2827/2928 (97%)	2796 (99%)	31 (1%)	65	84

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

Mol	Chain	Res	Type
1	A	35	ARG
1	A	67	VAL
1	A	220	ASP
2	B	70	PHE
3	C	6	ILE
4	D	132	ASN
5	E	185	CYS
1	F	35	ARG
1	F	67	VAL
2	G	70	PHE
4	I	108	SER
4	I	132	ASN
4	I	141	ARG
5	J	185	CYS
1	K	35	ARG
1	K	67	VAL
2	L	70	PHE
3	M	6	ILE
4	N	11	LEU
4	N	108	SER
4	N	132	ASN
5	O	185	CYS
1	P	35	ARG
1	P	67	VAL
2	Q	19	LYS
2	Q	70	PHE
3	R	6	ILE
4	S	11	LEU
4	S	132	ASN

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Mol	Chain	Res	Type
5	T	19	MET
5	T	185	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	151	HIS
1	A	155	GLN
4	D	44	GLN
4	D	206	ASN
5	E	44	GLN
5	E	198	ASN
5	E	216	GLN
1	F	54	GLN
1	F	226	GLN
4	I	132	ASN
4	I	164	GLN
4	I	206	ASN
5	J	189	GLN
1	K	32	GLN
1	K	151	HIS
1	K	155	GLN
4	N	7	ASN
4	N	164	GLN
4	N	206	ASN
5	O	189	GLN
1	P	32	GLN
1	P	155	GLN
4	S	132	ASN
4	S	164	GLN
4	S	206	ASN
5	T	189	GLN
5	T	216	GLN

5.3.3 RNA ⓘ

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 ⓘ

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, 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	271/277 (97%)	-1.52	0 100 100	30, 45, 63, 84	0
1	F	274/277 (98%)	-1.50	0 100 100	27, 46, 72, 97	0
1	K	259/277 (93%)	-1.45	0 100 100	34, 54, 86, 101	0
1	P	271/277 (97%)	-1.48	0 100 100	33, 52, 81, 106	0
2	B	100/100 (100%)	-1.56	0 100 100	31, 46, 66, 71	0
2	G	100/100 (100%)	-1.50	0 100 100	30, 45, 68, 72	0
2	L	100/100 (100%)	-1.51	0 100 100	34, 50, 75, 81	0
2	Q	100/100 (100%)	-1.49	0 100 100	34, 48, 68, 72	0
3	C	9/9 (100%)	-1.61	0 100 100	31, 34, 37, 38	0
3	H	9/9 (100%)	-1.57	0 100 100	33, 37, 40, 45	0
3	M	9/9 (100%)	-1.53	0 100 100	33, 38, 45, 51	0
3	R	9/9 (100%)	-1.64	0 100 100	31, 37, 43, 43	0
4	D	194/206 (94%)	-1.45	0 100 100	32, 47, 81, 93	0
4	I	194/206 (94%)	-1.42	0 100 100	32, 48, 84, 95	0
4	N	188/206 (91%)	-1.45	0 100 100	32, 48, 80, 98	0
4	S	189/206 (91%)	-1.42	0 100 100	33, 49, 77, 91	0
5	E	239/244 (97%)	-1.53	0 100 100	32, 46, 71, 80	0
5	J	239/244 (97%)	-1.53	0 100 100	30, 47, 73, 87	0
5	O	237/244 (97%)	-1.48	0 100 100	32, 47, 87, 103	0
5	T	240/244 (98%)	-1.48	0 100 100	33, 49, 80, 96	0
All	All	3231/3344 (96%)	-1.49	0 100 100	27, 48, 78, 106	0

There are no RSRZ outliers to report.

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 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.