



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 02:14 PM EDT

PDB ID : 5W1W / pdb_00005w1w
Title : Structure of the HLA-E-VMAPRTLVL/GF4 TCR complex
Authors : Gras, S.; Walpole, N.; Farenc, C.; Rossjohn, J.
Deposited on : 2017-06-05
Resolution : 3.10 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	:	4-5-2 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

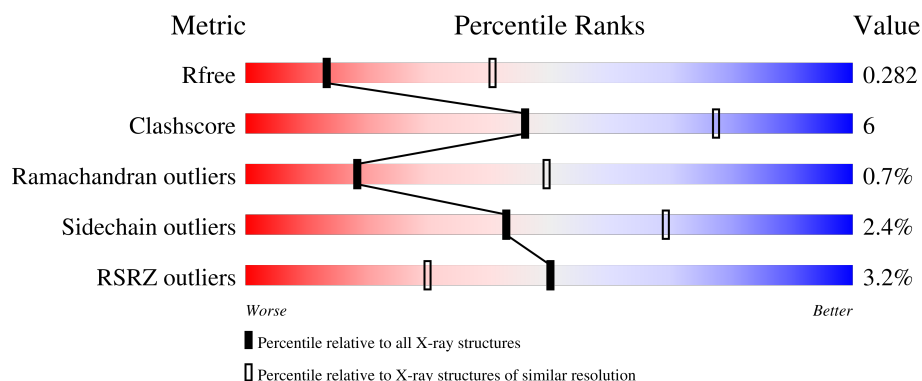
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	278	 83% 14% ..
1	F	278	 9% 80% 17% .
1	K	278	 4% 88% 10% .
1	P	278	 4% 85% 12% ..
2	B	100	 82% 18%

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Mol	Chain	Length	Quality of chain
2	G	100	
2	L	100	
2	Q	100	
3	C	9	
3	H	9	
3	M	9	
3	R	9	
4	D	207	
4	I	207	
4	N	207	
4	S	207	
5	E	246	
5	J	246	
5	O	246	
5	T	246	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26478 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, alpha chain E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2221	1392	398	424	7			
1	F	272	Total	C	N	O	S	0	0	0
			2221	1392	398	424	7			
1	K	272	Total	C	N	O	S	0	1	0
			2230	1397	399	427	7			
1	P	272	Total	C	N	O	S	0	1	0
			2230	1397	399	427	7			

- 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	1	0
			848	539	145	160	4			
2	G	100	Total	C	N	O	S	0	1	0
			848	539	145	160	4			
2	L	100	Total	C	N	O	S	0	1	0
			848	539	145	160	4			
2	Q	100	Total	C	N	O	S	0	1	0
			848	539	145	160	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 leader peptide of HLA class I histocompatibility antigen, A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			69	45	12	11	1			
3	H	9	Total	C	N	O	S	0	0	0
			69	45	12	11	1			
3	M	9	Total	C	N	O	S	0	0	0
			69	45	12	11	1			
3	R	9	Total	C	N	O	S	0	0	0
			69	45	12	11	1			

- Molecule 4 is a protein called GF4 T cell receptor alpha chain.

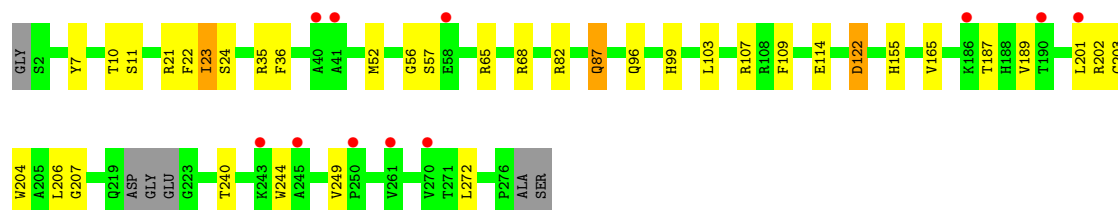
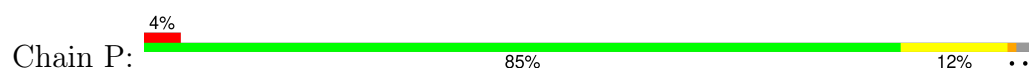
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	201	Total	C	N	O	S	0	0	0
			1551	975	253	314	9			
4	I	202	Total	C	N	O	S	0	0	0
			1560	980	255	316	9			
4	N	199	Total	C	N	O	S	0	0	0
			1537	967	251	311	8			
4	S	202	Total	C	N	O	S	0	0	0
			1556	978	254	315	9			

- Molecule 5 is a protein called GF4 T cell receptor beta chain.

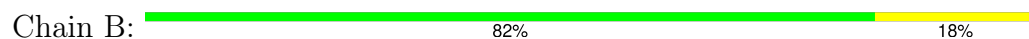
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1926	1213	334	374	5			
5	J	243	Total	C	N	O	S	0	0	0
			1926	1213	334	374	5			
5	O	243	Total	C	N	O	S	0	0	0
			1926	1213	334	374	5			
5	T	243	Total	C	N	O	S	0	0	0
			1926	1213	334	374	5			

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

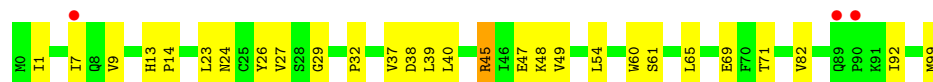




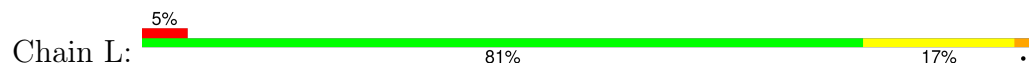
- Molecule 2: Beta-2-microglobulin



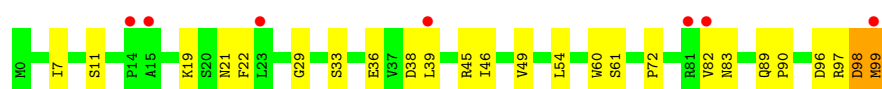
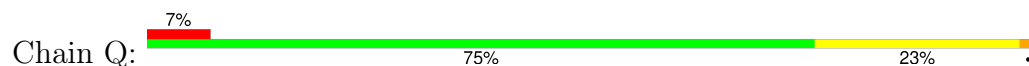
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- Molecule 2: Beta-2-microglobulin



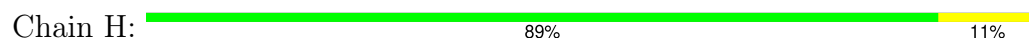
- Molecule 2: Beta-2-microglobulin



- Molecule 3: leader peptide of HLA class I histocompatibility antigen, A alpha chain



- Molecule 3: leader peptide of HLA class I histocompatibility antigen, A alpha chain

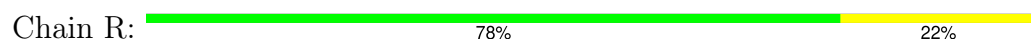




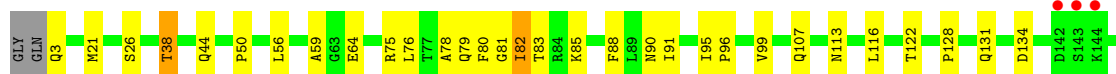
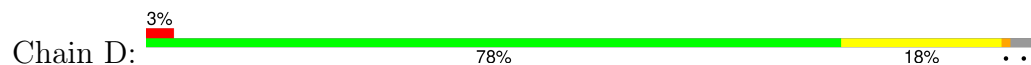
- Molecule 3: leader peptide of HLA class I histocompatibility antigen, A alpha chain



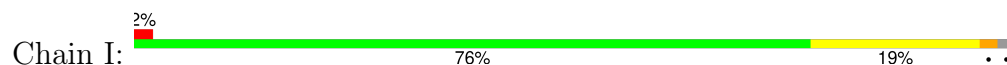
- Molecule 3: leader peptide of HLA class I histocompatibility antigen, A alpha chain



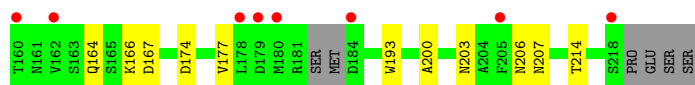
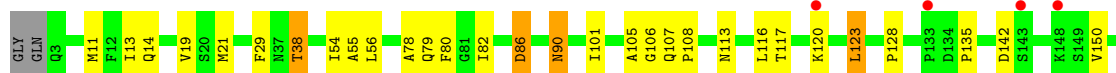
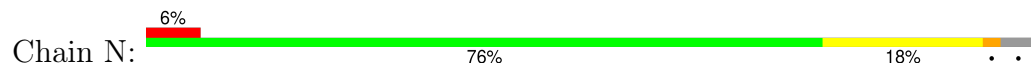
- Molecule 4: GF4 T cell receptor alpha chain



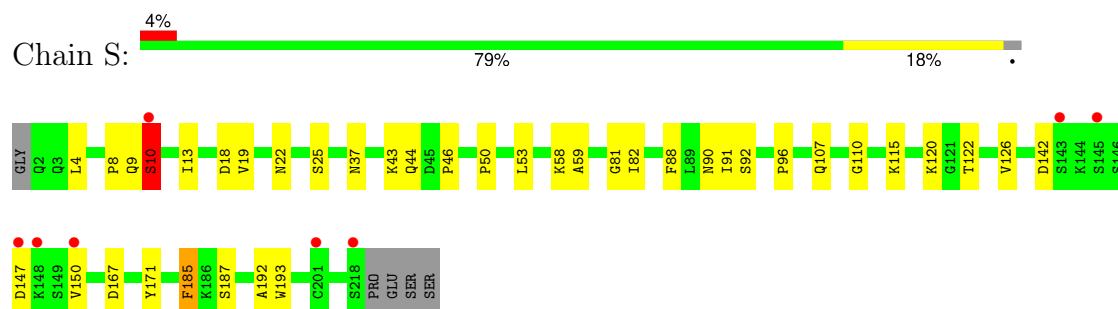
- Molecule 4: GF4 T cell receptor alpha chain



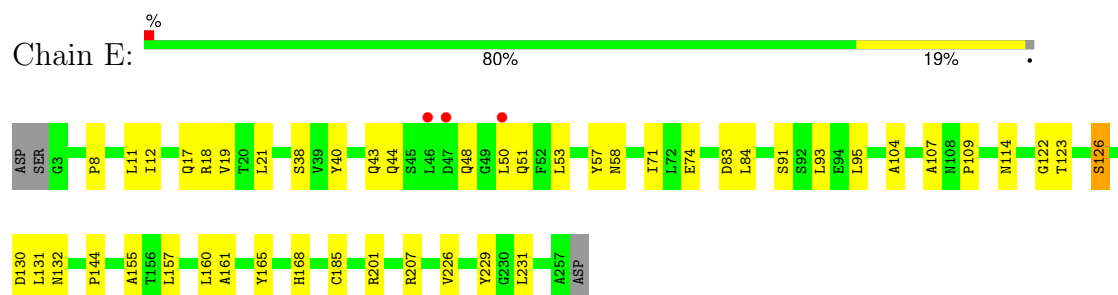
- Molecule 4: GF4 T cell receptor alpha chain



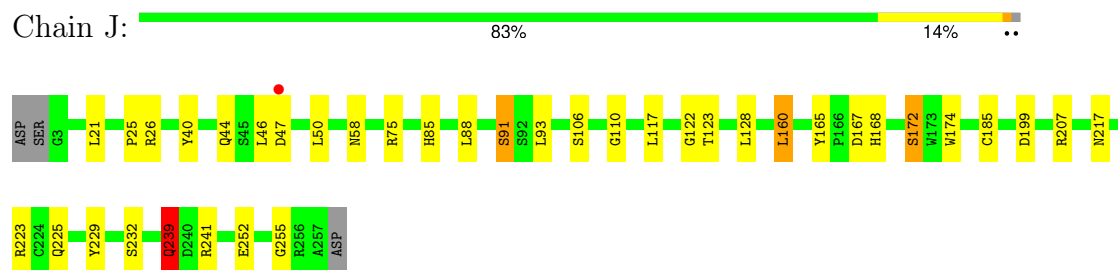
- Molecule 4: GF4 T cell receptor alpha chain



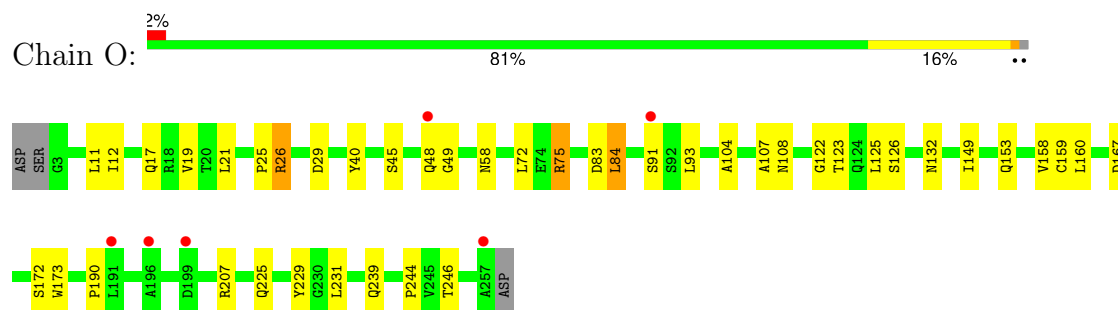
- Molecule 5: GF4 T cell receptor beta chain



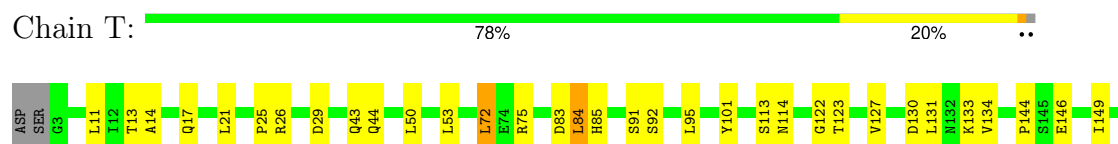
- Molecule 5: GF4 T cell receptor beta chain



- Molecule 5: GF4 T cell receptor beta chain



- Molecule 5: GF4 T cell receptor 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	73.37Å 225.93Å 276.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.29 – 3.10 50.29 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.29-3.10) 99.8 (50.29-3.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.215 , 0.263 0.230 , 0.282	Depositor DCC
R_{free} test set	4202 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	26478	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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	0.67	0/2287	1.29	6/3110 (0.2%)
1	F	0.72	0/2287	1.30	5/3110 (0.2%)
1	K	0.70	1/2296 (0.0%)	1.29	1/3122 (0.0%)
1	P	0.74	0/2296	1.27	5/3122 (0.2%)
2	B	0.66	0/871	1.18	3/1176 (0.3%)
2	G	0.68	0/871	1.22	3/1176 (0.3%)
2	L	0.72	0/871	1.18	3/1176 (0.3%)
2	Q	0.75	0/871	1.22	2/1176 (0.2%)
3	C	0.69	0/69	0.98	0/92
3	H	0.75	0/69	0.87	0/92
3	M	0.67	0/69	0.96	0/92
3	R	0.62	0/69	0.90	0/92
4	D	0.72	0/1585	1.25	5/2151 (0.2%)
4	I	0.72	0/1594	1.21	4/2163 (0.2%)
4	N	0.70	0/1570	1.20	6/2130 (0.3%)
4	S	0.75	0/1590	1.23	11/2158 (0.5%)
5	E	0.65	0/1976	1.22	1/2689 (0.0%)
5	J	0.65	0/1976	1.22	11/2689 (0.4%)
5	O	0.67	0/1976	1.21	2/2689 (0.1%)
5	T	0.66	0/1976	1.20	9/2689 (0.3%)
All	All	0.69	1/27169 (0.0%)	1.24	77/36894 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	249	VAL	CA-C	5.01	1.56	1.52

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	83	ASP	N-CA-C	-9.15	95.26	109.25
5	O	83	ASP	N-CA-C	-8.87	95.68	109.25
5	T	83	ASP	N-CA-C	-7.41	97.92	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	71	THR	CB-CA-C	6.95	117.42	110.33
1	F	197	HIS	CB-CA-C	-6.59	99.22	110.88

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	2221	0	2066	22	0
1	F	2221	0	2066	26	0
1	K	2230	0	2071	16	0
1	P	2230	0	2071	27	0
2	B	848	0	815	8	0
2	G	848	0	815	14	0
2	L	848	0	815	12	0
2	Q	848	0	814	36	0
3	C	69	0	83	2	0
3	H	69	0	83	0	0
3	M	69	0	83	2	0
3	R	69	0	83	1	0
4	D	1551	0	1481	22	0
4	I	1560	0	1489	26	0
4	N	1537	0	1466	23	0
4	S	1556	0	1483	21	0
5	E	1926	0	1828	25	0
5	J	1926	0	1828	17	0
5	O	1926	0	1828	26	0
5	T	1926	0	1828	24	0
All	All	26478	0	25096	301	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 6.

The worst 5 of 301 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:96:ASP:OD1	2:Q:99:MET:N	1.59	1.34
1:P:244:TRP:CZ2	2:Q:99:MET:HE1	1.73	1.24
2:Q:96:ASP:CG	2:Q:99:MET:HA	1.61	1.24
2:Q:96:ASP:OD1	2:Q:99:MET:CA	1.98	1.11
1:P:244:TRP:CH2	2:Q:99:MET:HE1	1.97	1.00

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	268/278 (96%)	248 (92%)	20 (8%)	0	100	100
1	F	268/278 (96%)	243 (91%)	23 (9%)	2 (1%)	18	49
1	K	269/278 (97%)	244 (91%)	24 (9%)	1 (0%)	30	61
1	P	269/278 (97%)	252 (94%)	16 (6%)	1 (0%)	30	61
2	B	99/100 (99%)	97 (98%)	2 (2%)	0	100	100
2	G	99/100 (99%)	95 (96%)	4 (4%)	0	100	100
2	L	99/100 (99%)	93 (94%)	6 (6%)	0	100	100
2	Q	99/100 (99%)	96 (97%)	3 (3%)	0	100	100
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%)	7 (100%)	0	0	100	100
4	D	199/207 (96%)	184 (92%)	13 (6%)	2 (1%)	12	41
4	I	200/207 (97%)	185 (92%)	14 (7%)	1 (0%)	24	57
4	N	195/207 (94%)	176 (90%)	18 (9%)	1 (0%)	24	57
4	S	200/207 (97%)	182 (91%)	15 (8%)	3 (2%)	8	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	241/246 (98%)	221 (92%)	18 (8%)	2 (1%)	16	47
5	J	241/246 (98%)	220 (91%)	16 (7%)	5 (2%)	5	25
5	O	241/246 (98%)	218 (90%)	20 (8%)	3 (1%)	10	37
5	T	241/246 (98%)	222 (92%)	16 (7%)	3 (1%)	10	37
All	All	3256/3360 (97%)	3001 (92%)	231 (7%)	24 (1%)	18	49

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	84	LEU
5	J	122	GLY
1	K	107	ARG
5	T	122	GLY
4	D	181	ARG

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	235/239 (98%)	232 (99%)	3 (1%)	61	77
1	F	235/239 (98%)	232 (99%)	3 (1%)	61	77
1	K	236/239 (99%)	232 (98%)	4 (2%)	53	74
1	P	236/239 (99%)	231 (98%)	5 (2%)	47	71
2	B	96/95 (101%)	93 (97%)	3 (3%)	35	64
2	G	96/95 (101%)	94 (98%)	2 (2%)	47	71
2	L	96/95 (101%)	94 (98%)	2 (2%)	47	71
2	Q	96/95 (101%)	92 (96%)	4 (4%)	26	58
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	19
3	H	8/8 (100%)	7 (88%)	1 (12%)	4	19
3	M	8/8 (100%)	7 (88%)	1 (12%)	4	19
3	R	8/8 (100%)	7 (88%)	1 (12%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	178/183 (97%)	171 (96%)	7 (4%)	28	60
4	I	179/183 (98%)	175 (98%)	4 (2%)	45	71
4	N	176/183 (96%)	170 (97%)	6 (3%)	32	63
4	S	178/183 (97%)	176 (99%)	2 (1%)	65	78
5	E	211/214 (99%)	204 (97%)	7 (3%)	33	63
5	J	211/214 (99%)	205 (97%)	6 (3%)	38	66
5	O	211/214 (99%)	208 (99%)	3 (1%)	59	76
5	T	211/214 (99%)	205 (97%)	6 (3%)	38	66
All	All	2913/2956 (98%)	2842 (98%)	71 (2%)	43	69

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	203	CYS
2	Q	89	GLN
5	T	11	LEU
2	G	45	ARG
1	F	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
2	Q	42	ASN
4	S	107	GLN
5	T	168	HIS
2	G	31	HIS
2	G	24	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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	272/278 (97%)	-0.01	4 (1%) 72 52	28, 57, 115, 136	0
1	F	272/278 (97%)	0.75	24 (8%) 15 9	41, 82, 147, 163	0
1	K	272/278 (97%)	0.54	10 (3%) 45 25	40, 95, 163, 176	1 (0%)
1	P	272/278 (97%)	0.52	11 (4%) 42 23	49, 99, 170, 185	1 (0%)
2	B	100/100 (100%)	-0.01	0 100 100	33, 58, 84, 99	1 (1%)
2	G	100/100 (100%)	0.78	3 (3%) 52 31	49, 92, 122, 134	1 (1%)
2	L	100/100 (100%)	0.72	5 (5%) 34 18	66, 124, 147, 155	1 (1%)
2	Q	100/100 (100%)	0.91	7 (7%) 22 12	68, 132, 154, 158	1 (1%)
3	C	9/9 (100%)	-0.43	0 100 100	30, 36, 39, 48	0
3	H	9/9 (100%)	-0.03	0 100 100	41, 47, 54, 56	0
3	M	9/9 (100%)	0.11	0 100 100	59, 61, 66, 83	0
3	R	9/9 (100%)	0.18	0 100 100	67, 69, 77, 90	0
4	D	201/207 (97%)	0.03	6 (2%) 52 31	26, 52, 119, 131	0
4	I	202/207 (97%)	-0.00	5 (2%) 58 37	27, 51, 114, 131	0
4	N	199/207 (96%)	0.63	12 (6%) 27 15	45, 74, 152, 158	0
4	S	202/207 (97%)	0.24	8 (3%) 42 23	42, 59, 118, 127	0
5	E	243/246 (98%)	-0.04	3 (1%) 76 58	29, 57, 92, 108	0
5	J	243/246 (98%)	-0.09	1 (0%) 88 76	35, 53, 86, 109	0
5	O	243/246 (98%)	0.43	6 (2%) 58 37	42, 81, 118, 129	0
5	T	243/246 (98%)	-0.08	0 100 100	28, 61, 93, 111	0
All	All	3300/3360 (98%)	0.29	105 (3%) 50 30	26, 72, 148, 185	6 (0%)

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	143	SER	3.6
1	F	261	VAL	3.5
4	N	180	MET	3.5
1	F	206	LEU	3.4
1	F	224	HIS	3.3

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.