



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 07:03 PM UTC

PDB ID : 1KTK / pdb_00001ktk
Title : Complex of Streptococcal pyrogenic enterotoxin C (SpeC) with a human T cell receptor beta chain (Vbeta2.1)
Authors : Sundberg, E.J.; Li, H.; Llera, A.S.; McCormick, J.K.; Tormo, J.; Karjalainen, K.; Schlievert, P.M.; Mariuzza, R.A.
Deposited on : 2002-01-16
Resolution : 3.00 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

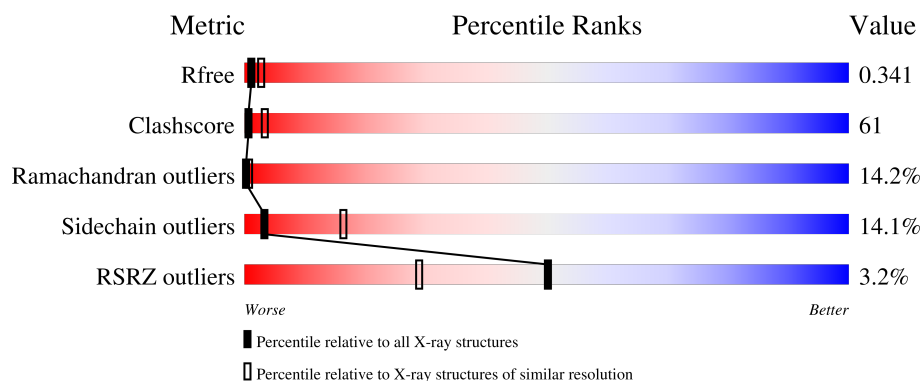
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	208	28% 50% 15% • •
1	B	208	3% 20% 60% 15% • •
1	C	208	29% 54% 14% •
1	D	208	33% 46% 14% • 5%
2	E	247	4% 18% 45% 28% 9%

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Mol	Chain	Length	Quality of chain
2	F	247	6%14%22%20%•42%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9511 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 Exotoxin type C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1664	1062	275	323	4			
1	B	200	Total	C	N	O	S	0	0	0
			1624	1042	267	311	4			
1	C	208	Total	C	N	O	S	0	0	0
			1699	1083	279	333	4			
1	D	198	Total	C	N	O	S	0	0	0
			1601	1028	267	303	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ASP	ASN	conflict	UNP P13380
B	26	ASP	ASN	conflict	UNP P13380
C	26	ASP	ASN	conflict	UNP P13380
D	26	ASP	ASN	conflict	UNP P13380

- Molecule 2 is a protein called T-cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	247	Total	C	N	O	S	0	0	0
			1879	1178	324	370	7			
2	F	144	Total	C	N	O	S	0	0	0
			1044	656	180	203	5			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	10	ARG	TRP	conflict	UNP P01850
E	13	ALA	CYS	conflict	UNP P01850
E	50	ALA	ASN	conflict	UNP P01850
E	95	LEU	-	insertion	UNP P01850

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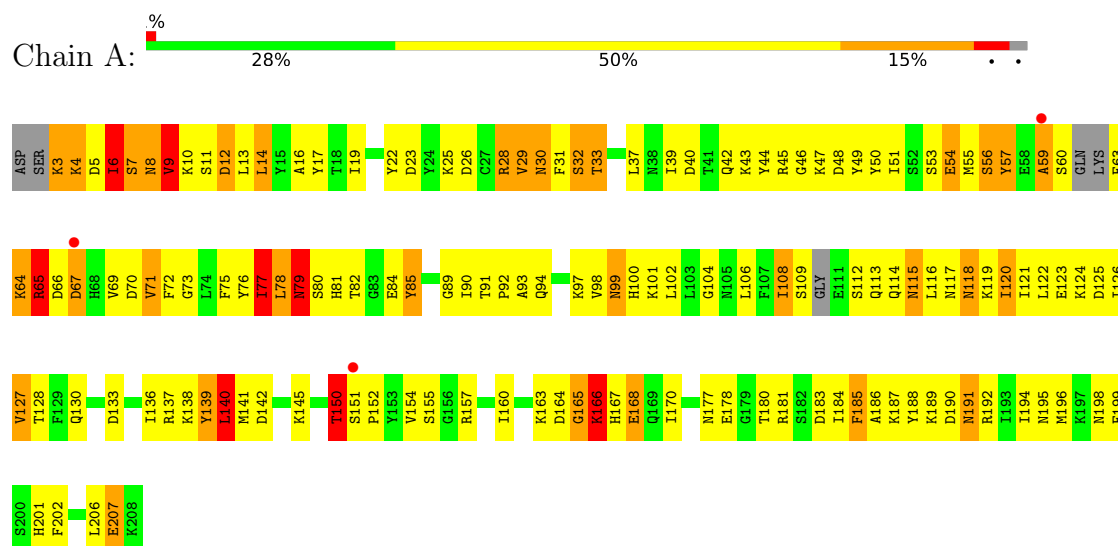
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Chain	Residue	Modelled	Actual	Comment	Reference
E	96	ALA	ARG	conflict	UNP P01850
E	99	GLY	GLU	conflict	UNP P01850
E	99	GLY	THR	conflict	UNP P01850
E	101	SER	-	insertion	UNP P01850
E	102	THR	-	insertion	UNP P01850
E	?	-	PRO	deletion	UNP P01850
E	?	-	LYS	deletion	UNP P01850
E	?	-	ASN	deletion	UNP P01850
E	105	THR	GLU	conflict	UNP P01850
E	107	TYR	PHE	conflict	UNP P01850
E	?	-	VAL	deletion	UNP P01850
E	191	ALA	CYS	conflict	UNP P01850
F	10	ARG	TRP	conflict	UNP P01850
F	13	ALA	CYS	conflict	UNP P01850
F	50	ALA	ASN	conflict	UNP P01850
F	96	LEU	-	insertion	UNP P01850
F	97	ALA	ARG	conflict	UNP P01850
F	98	GLY	GLU	conflict	UNP P01850
F	100	GLY	THR	conflict	UNP P01850
F	102	SER	-	insertion	UNP P01850
F	103	THR	-	insertion	UNP P01850
F	?	-	PRO	deletion	UNP P01850
F	?	-	LYS	deletion	UNP P01850
F	?	-	ASN	deletion	UNP P01850
F	105	THR	GLU	conflict	UNP P01850
F	107	TYR	PHE	conflict	UNP P01850
F	?	-	VAL	deletion	UNP P01850
F	191	ALA	CYS	conflict	UNP P01850

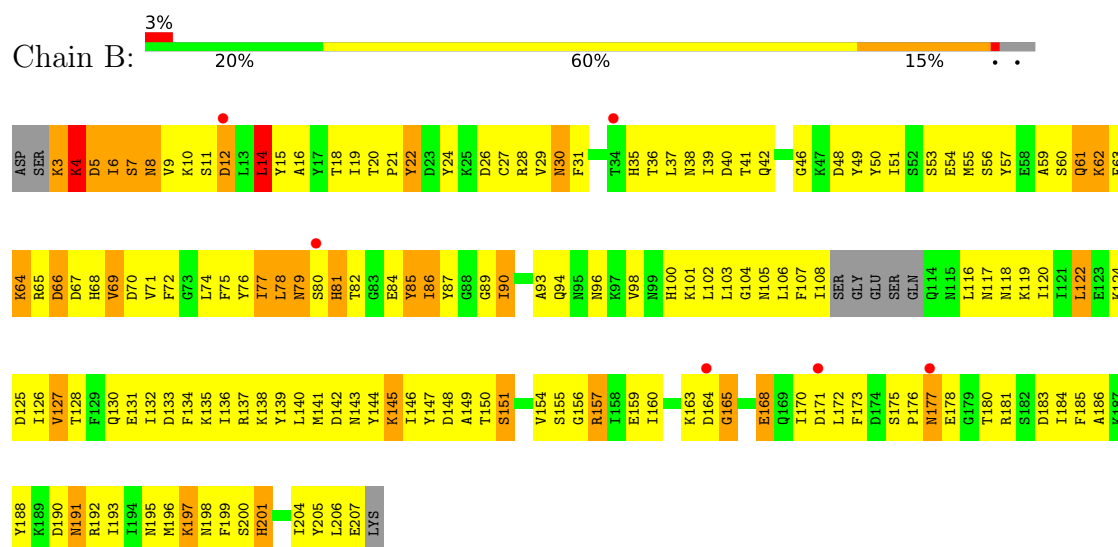
3 Residue-property plots

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: Exotoxin type C

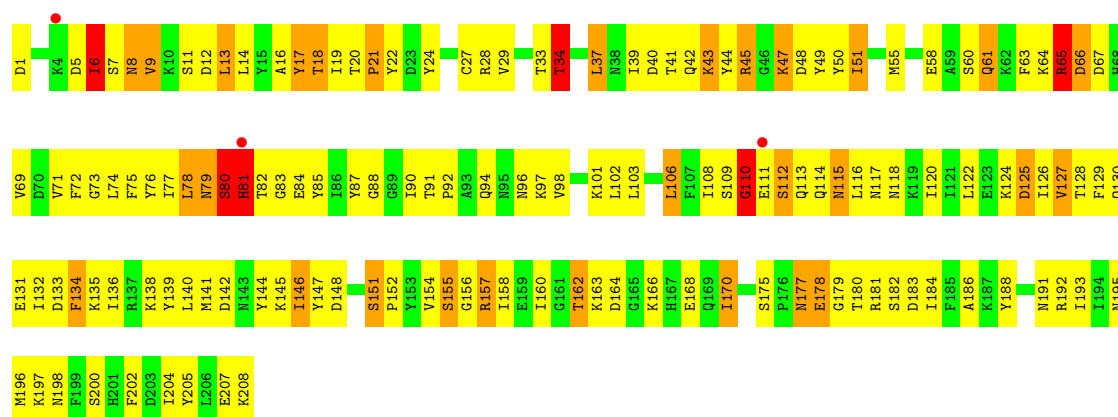


• Molecule 1: Exotoxin type C

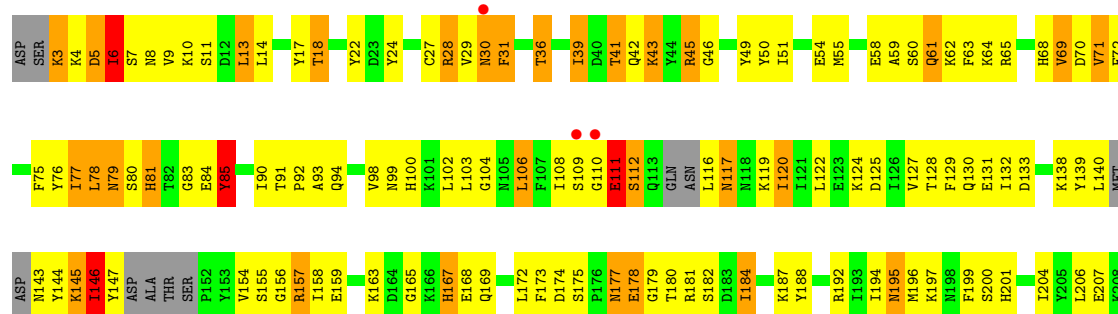


• Molecule 1: Exotoxin type C

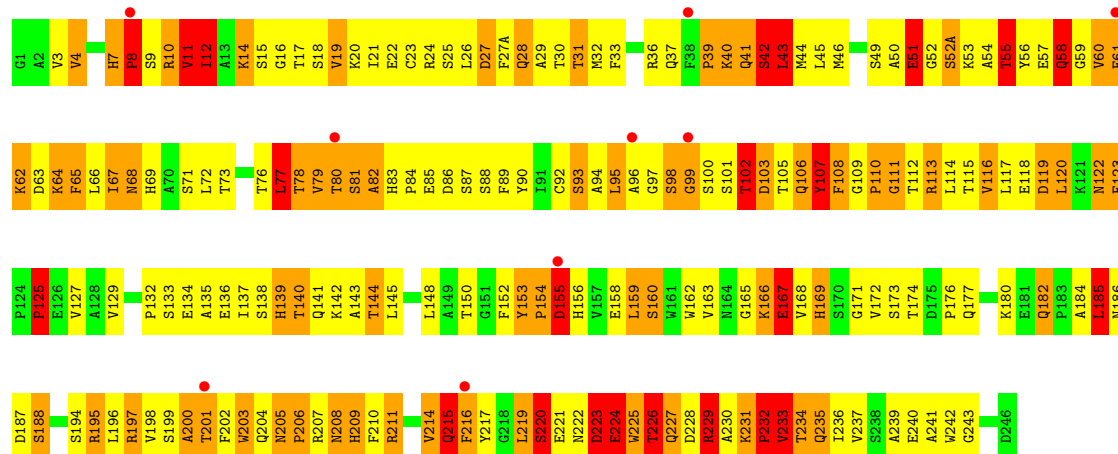
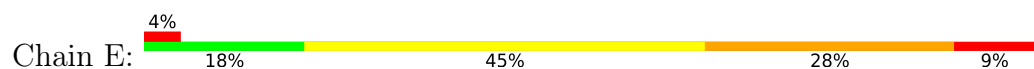




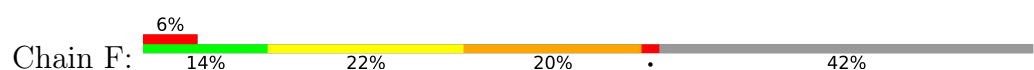
• Molecule 1: Exotoxin type C



• Molecule 2: T-cell receptor beta chain



• Molecule 2: T-cell receptor beta chain



GLY	GLN	ASP	TRP
ALA	GLN	PRO	GLY
VAL	PHE	ALA	ARG
V4	P124	LEU	ALA
S5	E126	N186	ASP
Q6	V127	S187	
H7	A128	S188	
P8	V129	R189	
S9	F130	Y190	
R10	E131	L191	
V11	P132	L192	
I12	SER	S193	
A13	GLU	S194	
K14	ALA	R195	
	GLU	L196	
T17	ILE	ARG	
S18	SER	VAL	
V19	HIS	SER	
K20	THR	ALA	
I21	GLN	THR	
E22	LYS	PHE	
C23	ALA	THR	
R24	THR	Q204	
	LEU	N205	
D27	V146	P206	
F27A	C147	R207	
Q28	L148	N208	
A29	A149	H209	
T30	T150	F210	
T31	Y90	R211	
M32	F152	CYS	
F33	TYR	GLN	
W34	PRO	V214	
Y35	ASP	Q215	
R36	HIS	F216	
Q37	VAL	Y217	
F38	GLY	GLY	
P39	LEU	LEU	
K40	SER	SER	
Q41	GLY	GLU	
S42	TRP	ASN	
L43	TRP	ASP	
M44	THR	GLU	
L45	ASP	TRP	
M46	THR	THR	
A47	GLN	GLN	
T48	F107	GLN	
S49	Y108	ASP	
A50	G109	ARG	
E51	P110	ALA	
G52	G111	LYS	
S52A	T112	PRO	
K53	R113	V233	
A54	L114	T234	
T55	T115	Q235	
TYR	V116	I236	
GLU	LEU	V237	
GLN	GLU	S238	
G59	ASP	A239	
V60	LEU	E240	
	LYS	ALA	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.38Å 146.76Å 135.69Å 90.00° 98.61° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00 6.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (6.00-3.00) 85.4 (6.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.326 , 0.334 0.334 , 0.341	Depositor DCC
R_{free} test set	1941 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	78.6	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.52 , 115.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	9511	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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	0.76	0/1697	1.28	17/2282 (0.7%)
1	B	0.59	0/1659	1.15	12/2240 (0.5%)
1	C	0.76	0/1735	1.23	23/2338 (1.0%)
1	D	0.60	0/1633	1.21	16/2197 (0.7%)
2	E	0.67	0/1924	1.52	38/2620 (1.5%)
2	F	0.55	0/1055	1.42	26/1421 (1.8%)
All	All	0.67	0/9703	1.31	132/13098 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

There are no bond length outliers.

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	7	HIS	CA-C-N	20.49	145.46	119.84
2	E	7	HIS	C-N-CA	20.49	145.46	119.84
1	D	80	SER	N-CA-C	-18.06	88.37	112.03
2	F	85	GLU	N-CA-C	-12.80	85.23	108.02
2	E	225	TRP	N-CA-C	12.22	127.78	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	130	PHE	Sidechain

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	1664	0	1608	193	0
1	B	1624	0	1554	224	0
1	C	1699	0	1634	150	0
1	D	1601	0	1539	165	0
2	E	1879	0	1775	306	1
2	F	1044	0	965	150	0
All	All	9511	0	9075	1142	1

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 61.

The worst 5 of 1142 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:E:57:GLU:OE2	2:E:63:ASP:HB2	1.43	1.17
1:A:180:THR:HG22	2:E:54:ALA:HB2	1.30	1.10
2:E:15:SER:HA	2:E:82:ALA:O	1.52	1.09
2:E:79:VAL:HG13	2:E:80:THR:H	1.17	1.08
2:F:86:ASP:HB3	2:F:115:THR:HA	1.15	1.08

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:141:GLN:OE1	2:E:223:ASP:OD2[1_655]	2.18	0.02

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	197/208 (95%)	145 (74%)	33 (17%)	19 (10%)	0	2
1	B	196/208 (94%)	146 (74%)	32 (16%)	18 (9%)	0	2
1	C	206/208 (99%)	152 (74%)	37 (18%)	17 (8%)	0	3
1	D	190/208 (91%)	147 (77%)	25 (13%)	18 (10%)	0	2
2	E	245/247 (99%)	143 (58%)	42 (17%)	60 (24%)	0	0
2	F	122/247 (49%)	59 (48%)	31 (25%)	32 (26%)	0	0
All	All	1156/1326 (87%)	792 (68%)	200 (17%)	164 (14%)	0	1

5 of 164 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	9	VAL
1	A	65	ARG
1	A	66	ASP
1	A	80	SER

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	183/192 (95%)	151 (82%)	32 (18%)	2	10
1	B	175/192 (91%)	159 (91%)	16 (9%)	9	33
1	C	186/192 (97%)	166 (89%)	20 (11%)	6	26
1	D	171/192 (89%)	155 (91%)	16 (9%)	8	32
2	E	201/213 (94%)	161 (80%)	40 (20%)	1	7
2	F	108/213 (51%)	88 (82%)	20 (18%)	1	9
All	All	1024/1194 (86%)	880 (86%)	144 (14%)	3	16

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	208	ASN
2	F	192	LEU
2	E	226	THR
2	F	61	GLU
1	C	1	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	28	GLN
2	E	208	ASN
2	E	37	GLN
2	E	141	GLN
2	E	227	GLN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	129:VAL	C	130:PHE	N	2.76

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	203/208 (97%)	-0.43	3 (1%)	72 49	29, 56, 87, 119	0
1	B	200/208 (96%)	-0.09	6 (3%)	52 30	49, 81, 103, 124	0
1	C	208/208 (100%)	-0.45	3 (1%)	73 51	34, 57, 84, 104	0
1	D	198/208 (95%)	-0.12	3 (1%)	72 49	50, 74, 110, 130	0
2	E	247/247 (100%)	0.13	9 (3%)	46 26	42, 80, 119, 130	0
2	F	144/247 (58%)	0.73	14 (9%)	13 7	69, 112, 137, 149	0
All	All	1200/1326 (90%)	-0.07	38 (3%)	50 29	29, 74, 123, 149	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	9	SER	4.1
1	D	110	GLY	3.7
2	F	239	ALA	3.4
2	F	208	ASN	3.4
2	F	233	VAL	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.