



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 03:46 pm BST

PDB ID : 5YXU
Title : an affinity enhanced T cell receptor in complex with HLA-A0201 restricted HCV NS3 peptide KLVALGINAV
Authors : Yi, L.
Deposited on : 2017-12-07
Resolution : 2.70 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 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 : 2.11
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) : 2.11

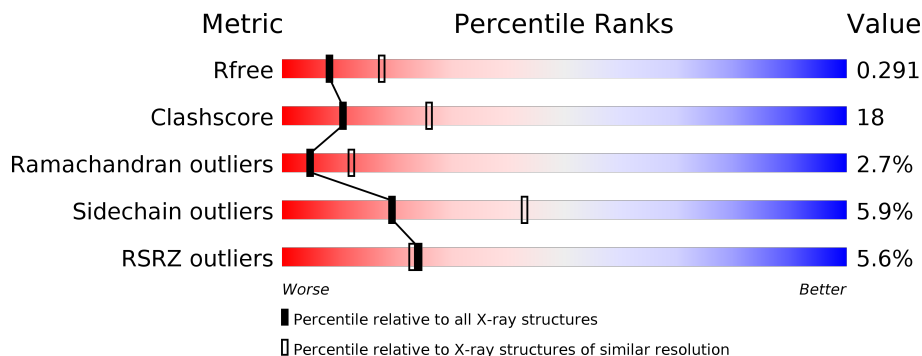
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



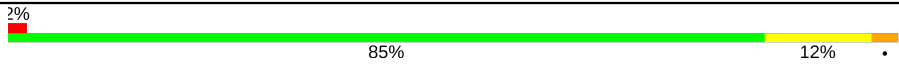

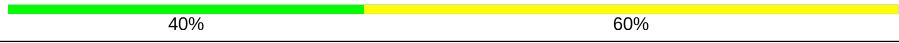

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	191	
1	F	191	
2	B	242	
2	G	242	
3	C	276	
3	E	276	

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Mol	Chain	Length	Quality of chain
4	D	100	 2% 85% 12% •
4	H	100	 2% 82% 16% ••
5	I	10	 40% 60%
5	J	10	 80% 20%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 13276 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 T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	F	190	Total 1506	C 939	N 251	O 306	S 10	0	0	0
1	A	191	Total 1515	C 944	N 253	O 308	S 10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	239	Total 1902	C 1198	N 329	O 367	S 8	0	0	0
2	B	242	Total 1931	C 1214	N 336	O 373	S 8	0	0	0

- Molecule 3 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	275	Total 2231	C 1394	N 405	O 423	S 9	0	0	0
3	E	276	Total 2233	C 1396	N 405	O 423	S 9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	277	ALA	-	expression tag	UNP P01892
E	277	ALA	-	expression tag	UNP P01892

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	100	Total 815	C 518	N 139	O 155	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	99	Total	C	N	O	S	0	0	0
			823	523	139	159	2			

- Molecule 5 is a protein called LYS-LEU-VAL-ALA-LEU-GLY-ILE-ASN-ALA-VAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	10	Total	C	N	O	0	0	0
			69	46	12	11			
5	J	10	Total	C	N	O	0	0	0
			69	46	12	11			

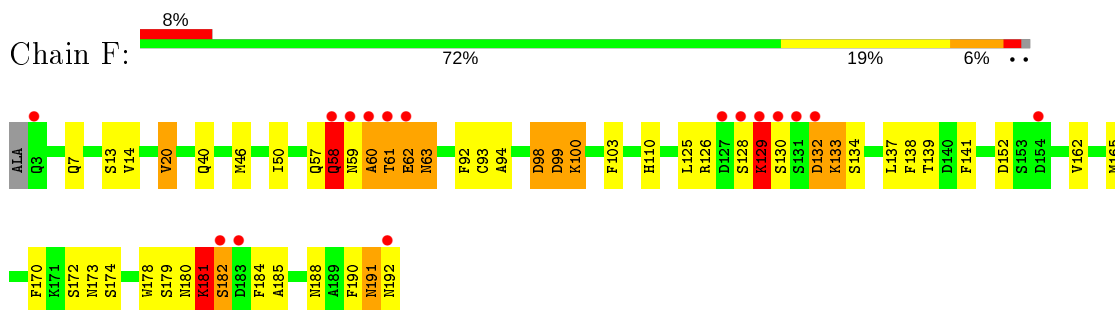
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	23	Total	O	0	0
			23	23		
6	G	30	Total	O	0	0
			30	30		
6	A	17	Total	O	0	0
			17	17		
6	B	24	Total	O	0	0
			24	24		
6	C	31	Total	O	0	0
			31	31		
6	D	14	Total	O	0	0
			14	14		
6	E	31	Total	O	0	0
			31	31		
6	H	10	Total	O	0	0
			10	10		
6	I	2	Total	O	0	0
			2	2		

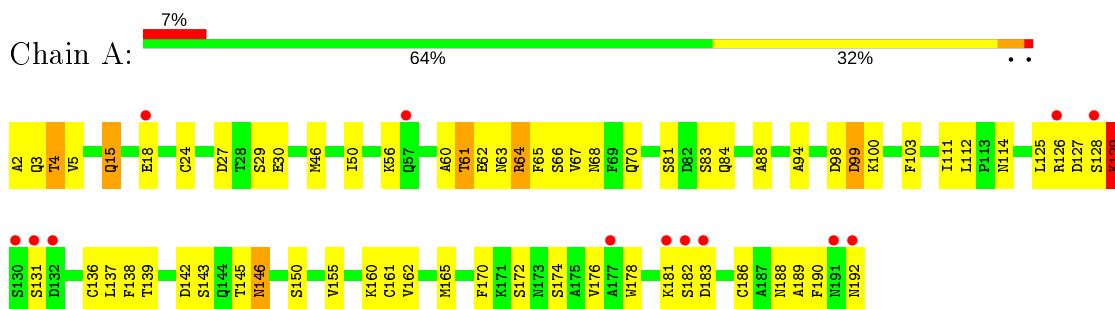
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

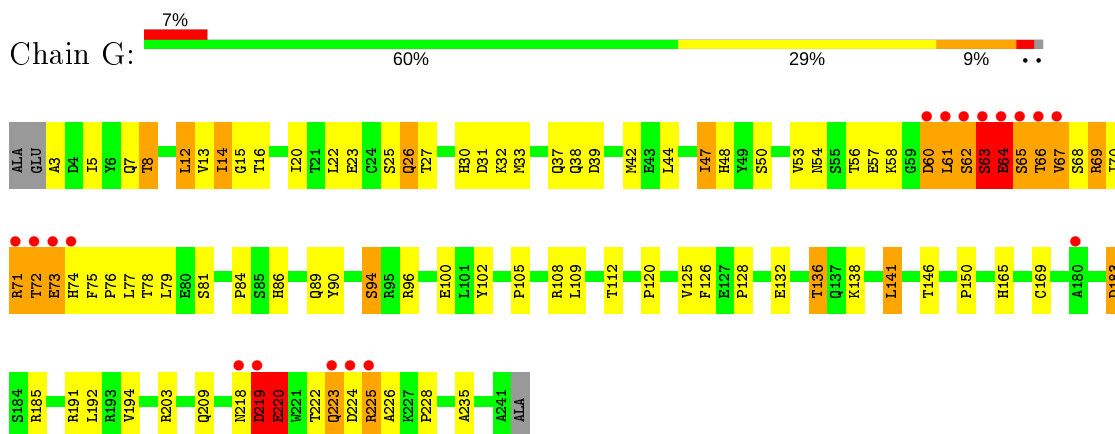
- Molecule 1: T cell receptor alpha chain



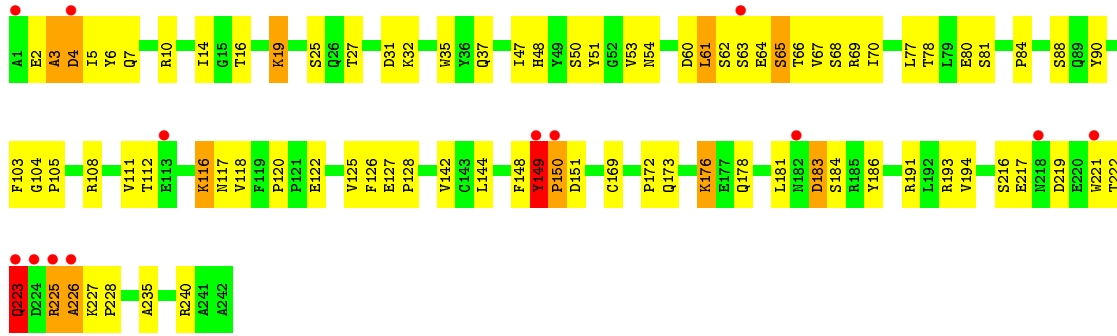
- Molecule 1: T cell receptor alpha chain



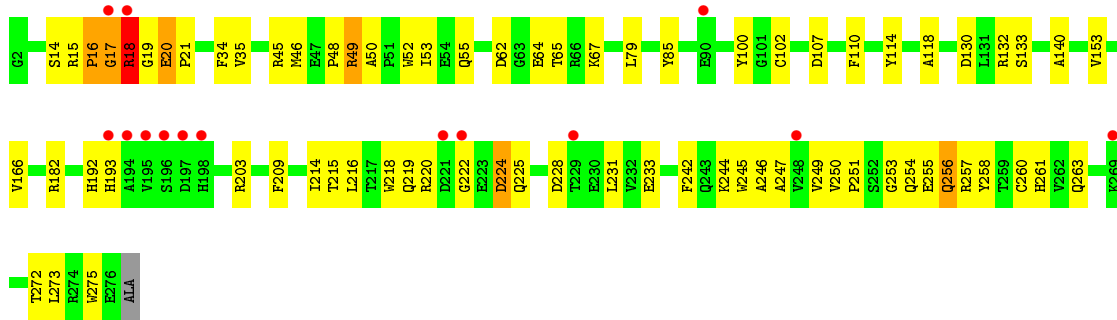
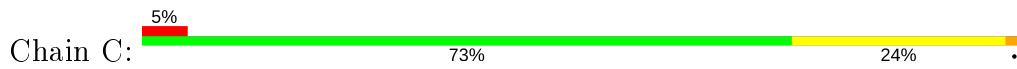
- Molecule 2: T cell receptor beta chain



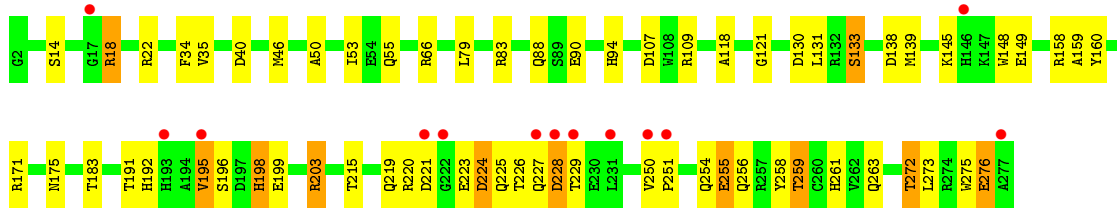
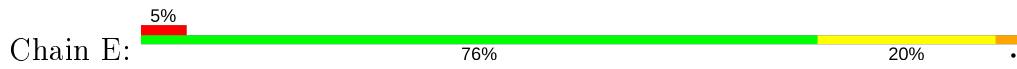
- Molecule 2: T cell receptor beta chain



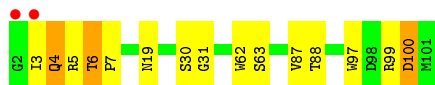
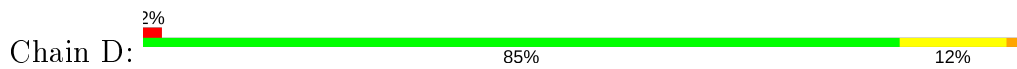
• Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain



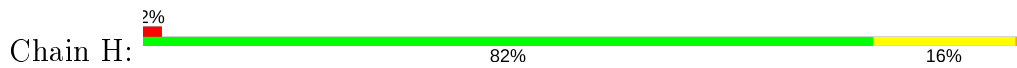
• Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain

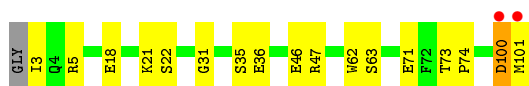


• Molecule 4: Beta-2-microglobulin



• Molecule 4: Beta-2-microglobulin

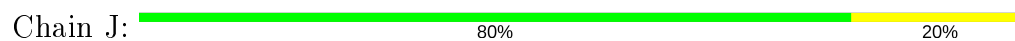




- Molecule 5: LYS-LEU-VAL-ALA-LEU-GLY-ILE-ASN-ALA-VAL



- Molecule 5: LYS-LEU-VAL-ALA-LEU-GLY-ILE-ASN-ALA-VAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.11Å 223.11Å 71.86Å 90.00° 98.30° 90.00°	Depositor
Resolution (Å)	17.70 – 2.70 17.73 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (17.70-2.70) 99.8 (17.73-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.235 , 0.289 0.243 , 0.291	Depositor DCC
R_{free} test set	2583 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtrriage
Anisotropy	0.291	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	13276	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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	0.63	0/1544	0.74	0/2088
1	F	0.49	0/1535	0.68	0/2076
2	B	0.52	1/1984 (0.1%)	0.70	1/2701 (0.0%)
2	G	0.51	0/1955	0.69	1/2663 (0.0%)
3	C	0.52	1/2296 (0.0%)	0.69	0/3119
3	E	0.51	0/2298	0.71	0/3123
4	D	0.45	0/838	0.63	0/1134
4	H	0.44	0/846	0.61	0/1147
5	I	0.67	0/68	0.70	0/91
5	J	0.49	0/68	0.63	0/91
All	All	0.52	2/13432 (0.0%)	0.69	2/18233 (0.0%)

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
1	A	0	2
1	F	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	150	PRO	N-CD	5.21	1.55	1.47
3	C	102	CYS	CB-SG	-5.16	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	149	TYR	C-N-CD	5.64	140.25	128.40
2	G	141	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	LYS	Peptide
1	A	98	ASP	Peptide
1	F	98	ASP	Peptide

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	1515	0	1442	62	0
1	F	1506	0	1429	56	0
2	B	1931	0	1838	103	0
2	G	1902	0	1802	129	2
3	C	2231	0	2066	58	0
3	E	2233	0	2066	59	0
4	D	815	0	763	16	2
4	H	823	0	770	16	0
5	I	69	0	85	8	0
5	J	69	0	85	2	0
6	A	17	0	0	3	0
6	B	24	0	0	2	0
6	C	31	0	0	1	0
6	D	14	0	0	1	0
6	E	31	0	0	2	0
6	F	23	0	0	1	0
6	G	30	0	0	3	0
6	H	10	0	0	1	0
6	I	2	0	0	0	0
All	All	13276	0	12346	465	2

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 18.

The worst 5 of 465 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:G:63:SER:CB	2:G:86:HIS:NE2	1.82	1.40
2:G:37:GLN:OE1	2:G:61:LEU:CD2	1.69	1.40
2:G:63:SER:HB2	2:G:86:HIS:NE2	1.04	1.35
1:A:2:ALA:CB	1:A:27:ASP:OD2	1.82	1.27
1:A:136:CYS:CB	1:A:186:CYS:SG	2.23	1.27

All (2) 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:G:81:SER:CB	4:D:3:ILE:CD1[1_454]	1.86	0.34
2:G:81:SER:CB	4:D:3:ILE:CG1[1_454]	2.16	0.04

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	189/191 (99%)	166 (88%)	19 (10%)	4 (2%)	7	18
1	F	188/191 (98%)	162 (86%)	19 (10%)	7 (4%)	3	7
2	B	240/242 (99%)	212 (88%)	19 (8%)	9 (4%)	3	7
2	G	237/242 (98%)	201 (85%)	23 (10%)	13 (6%)	2	3
3	C	273/276 (99%)	254 (93%)	15 (6%)	4 (2%)	10	26
3	E	274/276 (99%)	257 (94%)	12 (4%)	5 (2%)	8	21
4	D	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
4	H	97/100 (97%)	90 (93%)	6 (6%)	1 (1%)	15	37
5	I	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
5	J	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	1612/1638 (98%)	1446 (90%)	123 (8%)	43 (3%)	5	12

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	129	LYS
1	F	191	ASN
2	G	60	ASP
2	G	64	GLU
2	G	65	SER

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	172/172 (100%)	163 (95%)	9 (5%)	23	49
1	F	171/172 (99%)	156 (91%)	15 (9%)	10	23
2	B	211/211 (100%)	200 (95%)	11 (5%)	23	49
2	G	208/211 (99%)	187 (90%)	21 (10%)	7	17
3	C	228/231 (99%)	215 (94%)	13 (6%)	20	44
3	E	227/231 (98%)	216 (95%)	11 (5%)	25	53
4	D	90/94 (96%)	86 (96%)	4 (4%)	28	56
4	H	92/94 (98%)	92 (100%)	0	100	100
5	I	7/7 (100%)	7 (100%)	0	100	100
5	J	7/7 (100%)	7 (100%)	0	100	100
All	All	1413/1430 (99%)	1329 (94%)	84 (6%)	19	43

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
2	B	67	VAL
3	E	198	HIS
1	A	61	THR
1	A	129	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	86	HIS
2	G	89	GLN
1	A	191	ASN
2	G	26	GLN
1	A	70	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 carbohydrates 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	191/191 (100%)	0.32	13 (6%) 17 15	15, 28, 68, 94	0
1	F	190/191 (99%)	0.38	16 (8%) 11 9	13, 27, 63, 84	0
2	B	242/242 (100%)	0.25	13 (5%) 25 24	13, 28, 59, 72	0
2	G	239/242 (98%)	0.19	18 (7%) 14 12	13, 21, 46, 68	0
3	C	275/276 (99%)	0.12	14 (5%) 28 26	11, 27, 59, 83	0
3	E	276/276 (100%)	0.17	13 (4%) 31 30	12, 26, 67, 93	0
4	D	100/100 (100%)	0.22	2 (2%) 65 67	14, 36, 55, 62	0
4	H	99/100 (99%)	0.12	2 (2%) 65 67	17, 32, 50, 60	0
5	I	10/10 (100%)	-0.63	0 100 100	14, 16, 19, 21	0
5	J	10/10 (100%)	-0.55	0 100 100	13, 17, 19, 22	0
All	All	1632/1638 (99%)	0.21	91 (5%) 24 23	11, 26, 60, 94	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	66	THR	12.9
2	G	65	SER	11.6
1	F	59	ASN	9.8
1	F	131	SER	7.7
1	A	182	SER	7.6

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 carbohydrates 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.