



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 01:28 pm BST

PDB ID : 6DWF
Title : Crystal structure of complex of BBKI mutant, L55R with Bovine Trypsin
Authors : Li, M.; Wlodawer, A.; Gustchina, A.
Deposited on : 2018-06-26
Resolution : 1.94 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

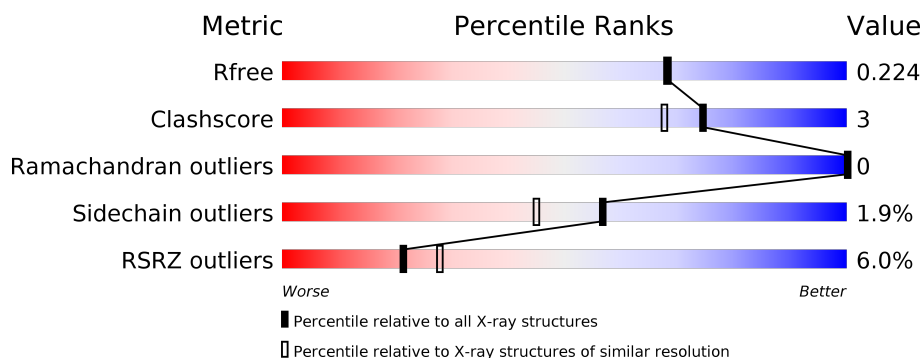
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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.





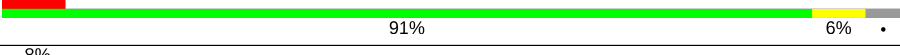

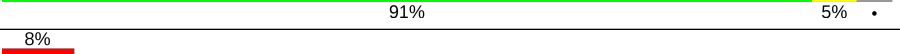
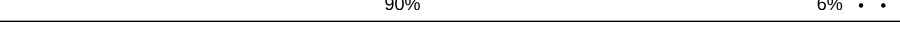
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	223	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	B	223	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	C	223	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	D	223	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
1	E	223	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	F	223	<div> <div>7%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	169	
2	H	169	
2	I	169	
2	J	169	
2	K	169	
2	L	169	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19041 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 Cationic trypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	1	0
			1631	1013	279	325	14			
1	B	223	Total	C	N	O	S	0	1	0
			1631	1013	279	325	14			
1	C	223	Total	C	N	O	S	0	1	0
			1631	1013	279	325	14			
1	D	223	Total	C	N	O	S	0	1	0
			1631	1013	279	325	14			
1	E	223	Total	C	N	O	S	0	1	0
			1631	1013	279	325	14			
1	F	223	Total	C	N	O	S	0	1	0
			1631	1013	279	325	14			

- Molecule 2 is a protein called Kunitz-type inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	163	Total	C	N	O	S	0	2	0
			1269	810	220	238	1			
2	H	163	Total	C	N	O	S	0	3	0
			1270	810	220	239	1			
2	I	163	Total	C	N	O	S	0	3	0
			1270	810	220	239	1			
2	J	163	Total	C	N	O	S	0	3	0
			1270	810	220	239	1			
2	K	163	Total	C	N	O	S	0	3	0
			1270	810	220	239	1			
2	L	163	Total	C	N	O	S	0	3	0
			1270	810	220	239	1			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-5	HIS	-	expression tag	UNP Q6VEQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	HIS	-	expression tag	UNP Q6VEQ7
G	-3	HIS	-	expression tag	UNP Q6VEQ7
G	-2	HIS	-	expression tag	UNP Q6VEQ7
G	-1	HIS	-	expression tag	UNP Q6VEQ7
G	0	HIS	-	expression tag	UNP Q6VEQ7
G	55	ARG	LEU	engineered mutation	UNP Q6VEQ7
H	-5	HIS	-	expression tag	UNP Q6VEQ7
H	-4	HIS	-	expression tag	UNP Q6VEQ7
H	-3	HIS	-	expression tag	UNP Q6VEQ7
H	-2	HIS	-	expression tag	UNP Q6VEQ7
H	-1	HIS	-	expression tag	UNP Q6VEQ7
H	0	HIS	-	expression tag	UNP Q6VEQ7
H	55	ARG	LEU	engineered mutation	UNP Q6VEQ7
I	-5	HIS	-	expression tag	UNP Q6VEQ7
I	-4	HIS	-	expression tag	UNP Q6VEQ7
I	-3	HIS	-	expression tag	UNP Q6VEQ7
I	-2	HIS	-	expression tag	UNP Q6VEQ7
I	-1	HIS	-	expression tag	UNP Q6VEQ7
I	0	HIS	-	expression tag	UNP Q6VEQ7
I	55	ARG	LEU	engineered mutation	UNP Q6VEQ7
J	-5	HIS	-	expression tag	UNP Q6VEQ7
J	-4	HIS	-	expression tag	UNP Q6VEQ7
J	-3	HIS	-	expression tag	UNP Q6VEQ7
J	-2	HIS	-	expression tag	UNP Q6VEQ7
J	-1	HIS	-	expression tag	UNP Q6VEQ7
J	0	HIS	-	expression tag	UNP Q6VEQ7
J	55	ARG	LEU	engineered mutation	UNP Q6VEQ7
K	-5	HIS	-	expression tag	UNP Q6VEQ7
K	-4	HIS	-	expression tag	UNP Q6VEQ7
K	-3	HIS	-	expression tag	UNP Q6VEQ7
K	-2	HIS	-	expression tag	UNP Q6VEQ7
K	-1	HIS	-	expression tag	UNP Q6VEQ7
K	0	HIS	-	expression tag	UNP Q6VEQ7
K	55	ARG	LEU	engineered mutation	UNP Q6VEQ7
L	-5	HIS	-	expression tag	UNP Q6VEQ7
L	-4	HIS	-	expression tag	UNP Q6VEQ7
L	-3	HIS	-	expression tag	UNP Q6VEQ7
L	-2	HIS	-	expression tag	UNP Q6VEQ7
L	-1	HIS	-	expression tag	UNP Q6VEQ7
L	0	HIS	-	expression tag	UNP Q6VEQ7
L	55	ARG	LEU	engineered mutation	UNP Q6VEQ7

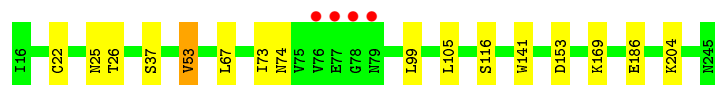
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total 133	O 133	0	0
3	G	117	Total 117	O 117	0	0
3	B	115	Total 115	O 115	0	0
3	C	135	Total 135	O 135	0	0
3	D	150	Total 150	O 150	0	0
3	E	166	Total 166	O 166	0	0
3	F	145	Total 145	O 145	0	0
3	H	130	Total 130	O 130	0	0
3	I	139	Total 139	O 139	0	0
3	J	122	Total 122	O 122	0	0
3	K	147	Total 147	O 147	0	0
3	L	137	Total 137	O 137	0	0

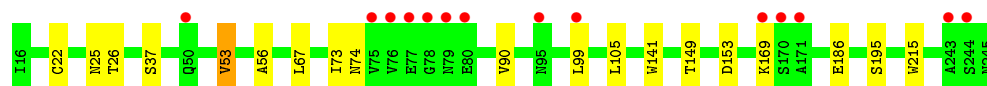
3 Residue-property plots [i](#)

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.

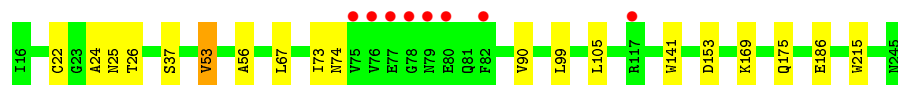
- Molecule 1: Cationic trypsin



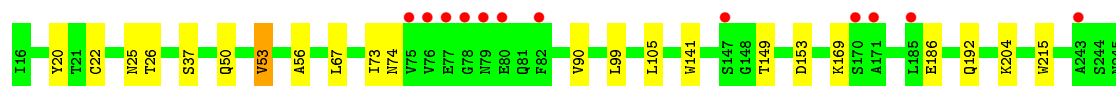
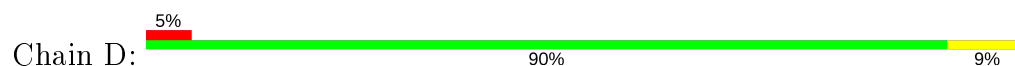
- Molecule 1: Cationic trypsin



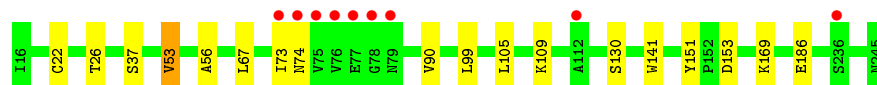
- Molecule 1: Cationic trypsin



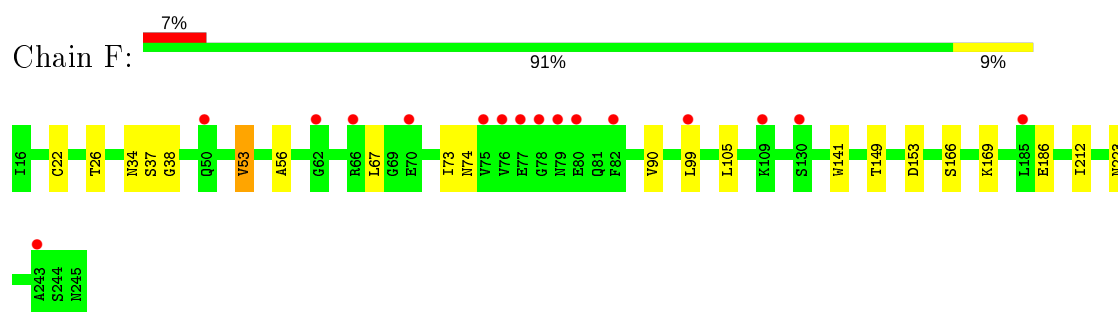
- Molecule 1: Cationic trypsin



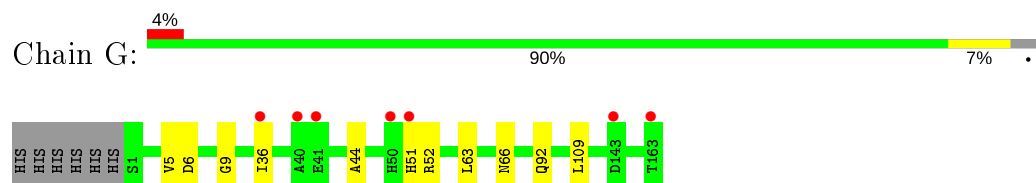
- Molecule 1: Cationic trypsin



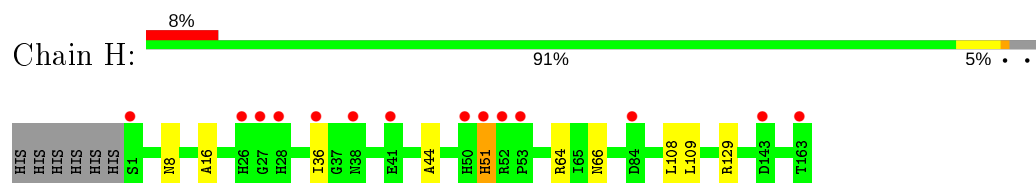
- Molecule 1: Cationic trypsin



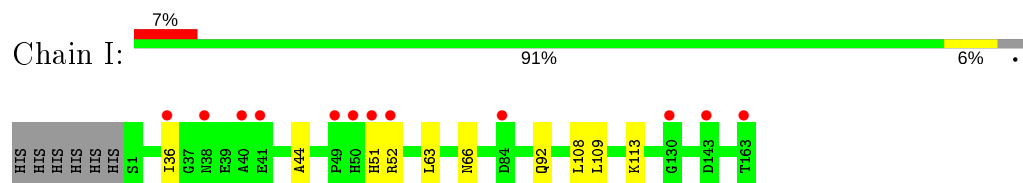
- Molecule 2: Kunitz-type inhibitor



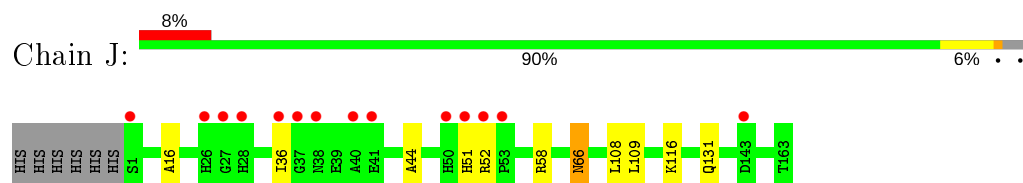
- Molecule 2: Kunitz-type inhibitor



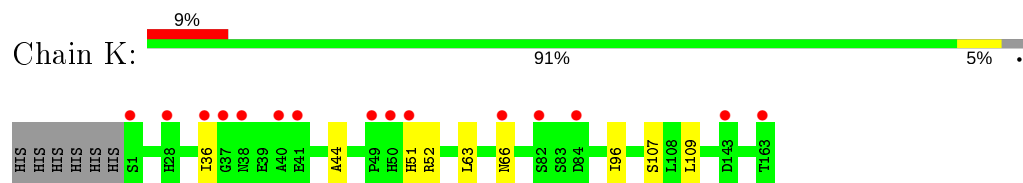
- Molecule 2: Kunitz-type inhibitor



- Molecule 2: Kunitz-type inhibitor



- Molecule 2: Kunitz-type inhibitor



- Molecule 2: Kunitz-type inhibitor





4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	207.30Å 207.30Å 107.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.79 – 1.94 49.79 – 1.94	Depositor EDS
% Data completeness (in resolution range)	88.3 (49.79-1.94) 88.3 (49.79-1.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.196 , 0.223 0.202 , 0.224	Depositor DCC
R_{free} test set	8111 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.492 for H, K, L 0.508 for -K, -H, -L	Depositor
Outliers	0 of 169855 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19041	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.77 % 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 6.7208e-06. 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

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	1/1666 (0.1%)	0.70	0/2258
1	B	0.61	1/1666 (0.1%)	0.69	0/2258
1	C	0.62	1/1666 (0.1%)	0.74	2/2258 (0.1%)
1	D	0.62	1/1666 (0.1%)	0.71	0/2258
1	E	0.64	1/1666 (0.1%)	0.71	0/2258
1	F	0.64	1/1666 (0.1%)	0.71	0/2258
2	G	0.48	0/1308	0.74	0/1776
2	H	0.47	0/1314	0.73	0/1784
2	I	0.47	0/1314	0.76	0/1784
2	J	0.49	0/1314	0.76	1/1784 (0.1%)
2	K	0.49	0/1314	0.75	0/1784
2	L	0.50	0/1314	0.76	1/1784 (0.1%)
All	All	0.57	6/17874 (0.0%)	0.73	4/24244 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	37	SER	CB-OG	-6.34	1.34	1.42
1	F	37	SER	CB-OG	-6.34	1.34	1.42
1	B	37	SER	CB-OG	-6.34	1.34	1.42
1	E	37	SER	CB-OG	-6.29	1.34	1.42
1	A	37	SER	CB-OG	-6.28	1.34	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	ALA	N-CA-C	-7.69	90.25	111.00
1	C	24	ALA	N-CA-CB	5.84	118.28	110.10
2	L	58	ARG	NE-CZ-NH1	5.41	123.00	120.30
2	J	58	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	1631	0	1589	13	0
1	B	1631	0	1589	16	0
1	C	1631	0	1589	15	0
1	D	1631	0	1589	19	0
1	E	1631	0	1589	11	0
1	F	1631	0	1589	14	0
2	G	1269	0	1272	11	0
2	H	1270	0	1273	10	0
2	I	1270	0	1273	10	0
2	J	1270	0	1273	12	0
2	K	1270	0	1273	9	0
2	L	1270	0	1273	11	0
3	A	133	0	0	0	0
3	B	115	0	0	1	1
3	C	135	0	0	1	0
3	D	150	0	0	1	0
3	E	166	0	0	3	0
3	F	145	0	0	6	0
3	G	117	0	0	5	0
3	H	130	0	0	2	0
3	I	139	0	0	2	0
3	J	122	0	0	1	1
3	K	147	0	0	0	0
3	L	137	0	0	2	0
All	All	19041	0	17171	111	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 3.

The worst 5 of 111 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)
1:A:26:THR:HG22	1:D:26:THR:HG22	1.30	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:THR:HG22	1:C:26:THR:HG22	1.41	1.00
2:G:6:ASP:O	3:G:201:HOH:O	1.92	0.86
1:E:130:SER:HB2	3:E:311:HOH:O	1.78	0.81
1:D:99:LEU:HD11	2:J:109:LEU:HD11	1.63	0.79

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)
3:B:386:HOH:O	3:J:204:HOH:O[2_655]	2.11	0.09

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	222/223 (100%)	218 (98%)	4 (2%)	0	100	100
1	B	222/223 (100%)	218 (98%)	4 (2%)	0	100	100
1	C	222/223 (100%)	217 (98%)	5 (2%)	0	100	100
1	D	222/223 (100%)	218 (98%)	4 (2%)	0	100	100
1	E	222/223 (100%)	218 (98%)	4 (2%)	0	100	100
1	F	222/223 (100%)	218 (98%)	4 (2%)	0	100	100
2	G	163/169 (96%)	156 (96%)	7 (4%)	0	100	100
2	H	164/169 (97%)	157 (96%)	7 (4%)	0	100	100
2	I	164/169 (97%)	157 (96%)	7 (4%)	0	100	100
2	J	164/169 (97%)	158 (96%)	6 (4%)	0	100	100
2	K	164/169 (97%)	157 (96%)	7 (4%)	0	100	100
2	L	164/169 (97%)	157 (96%)	7 (4%)	0	100	100
All	All	2315/2352 (98%)	2249 (97%)	66 (3%)	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	185/184 (100%)	181 (98%)	4 (2%)	52	39
1	B	185/184 (100%)	181 (98%)	4 (2%)	52	39
1	C	185/184 (100%)	181 (98%)	4 (2%)	52	39
1	D	185/184 (100%)	181 (98%)	4 (2%)	52	39
1	E	185/184 (100%)	181 (98%)	4 (2%)	52	39
1	F	185/184 (100%)	181 (98%)	4 (2%)	52	39
2	G	139/143 (97%)	137 (99%)	2 (1%)	67	58
2	H	140/143 (98%)	138 (99%)	2 (1%)	67	58
2	I	140/143 (98%)	138 (99%)	2 (1%)	67	58
2	J	140/143 (98%)	138 (99%)	2 (1%)	67	58
2	K	140/143 (98%)	136 (97%)	4 (3%)	42	28
2	L	140/143 (98%)	138 (99%)	2 (1%)	67	58
All	All	1949/1962 (99%)	1911 (98%)	38 (2%)	57	45

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	186	GLU
1	E	186	GLU
2	K	107[B]	SER
1	E	67	LEU
1	F	53	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	240	GLN

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Mol	Chain	Res	Type
1	D	34	ASN
2	I	66	ASN
1	C	34	ASN
1	F	34	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 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	223/223 (100%)	0.24	4 (1%) 68 74	10, 22, 41, 80	0
1	B	223/223 (100%)	0.48	14 (6%) 20 26	10, 27, 49, 82	0
1	C	223/223 (100%)	0.29	8 (3%) 42 50	12, 24, 41, 86	0
1	D	223/223 (100%)	0.38	12 (5%) 25 32	9, 24, 41, 83	0
1	E	223/223 (100%)	0.38	9 (4%) 38 45	10, 23, 39, 86	0
1	F	223/223 (100%)	0.62	16 (7%) 15 21	8, 25, 45, 84	0
2	G	163/169 (96%)	0.37	7 (4%) 35 42	9, 22, 50, 83	0
2	H	163/169 (96%)	0.41	14 (8%) 10 15	11, 24, 51, 66	0
2	I	163/169 (96%)	0.49	12 (7%) 14 20	12, 24, 54, 95	0
2	J	163/169 (96%)	0.41	14 (8%) 10 15	10, 22, 51, 66	0
2	K	163/169 (96%)	0.47	15 (9%) 9 13	10, 20, 47, 87	0
2	L	163/169 (96%)	0.39	13 (7%) 12 17	9, 20, 46, 58	0
All	All	2316/2352 (98%)	0.41	138 (5%) 21 28	8, 23, 49, 95	0

The worst 5 of 138 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	50	HIS	10.5
2	K	50	HIS	10.3
1	F	76	VAL	9.5
1	D	79	ASN	7.4
1	F	78	GLY	7.3

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 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.