



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:19 AM UTC

PDB ID : 5AJK / pdb_00005ajk
Title : Crystal structure of variola virus virulence factor F1L in complex with human Bak BH3 domain
Authors : Kvensakul, M.; Colman, P.M.
Deposited on : 2015-02-25
Resolution : 2.55 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
Mogul : 2022.3.0, CSD as543be (2022)
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

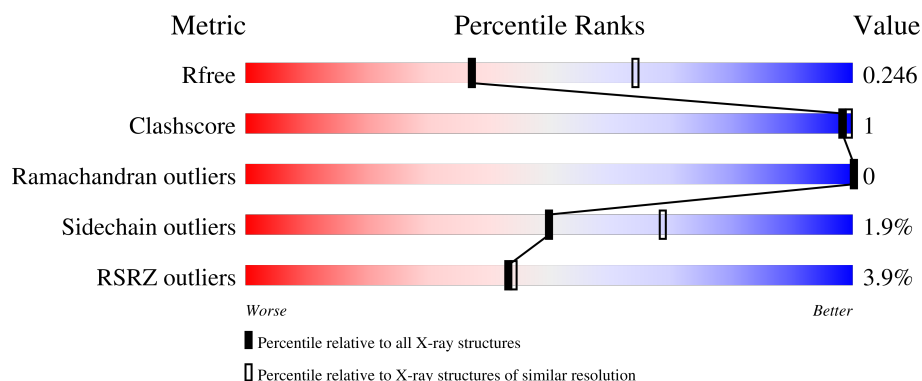
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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.



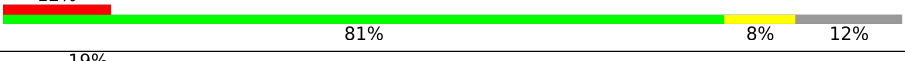
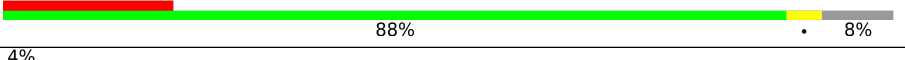
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	168	2% 84% 12%
1	C	168	0% 82% 17%
1	E	168	3% 80% 16%
1	G	168	0% 79% 18%
1	I	168	2% 79% 18%

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Mol	Chain	Length	Quality of chain
1	K	168	
2	B	26	
2	D	26	
2	F	26	
2	H	26	
2	J	26	
2	L	26	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15824 atoms, of which 7769 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 HOMOLOG OF VACCINIA VIRUS CDS F1L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	148	Total	C	H	N	O	S	0	0	0
			2386	763	1176	196	237	14			
1	C	139	Total	C	H	N	O	S	0	0	0
			2244	711	1110	184	225	14			
1	E	141	Total	C	H	N	O	S	0	0	0
			2290	732	1131	186	227	14			
1	G	137	Total	C	H	N	O	S	0	0	0
			2222	705	1100	182	221	14			
1	I	137	Total	C	H	N	O	S	0	0	0
			2219	704	1098	182	221	14			
1	K	138	Total	C	H	N	O	S	0	0	0
			2233	708	1105	183	223	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP Q85365
A	35	PRO	-	expression tag	UNP Q85365
A	36	LEU	-	expression tag	UNP Q85365
A	37	GLY	-	expression tag	UNP Q85365
A	38	SER	-	expression tag	UNP Q85365
C	34	GLY	-	expression tag	UNP Q85365
C	35	PRO	-	expression tag	UNP Q85365
C	36	LEU	-	expression tag	UNP Q85365
C	37	GLY	-	expression tag	UNP Q85365
C	38	SER	-	expression tag	UNP Q85365
E	34	GLY	-	expression tag	UNP Q85365
E	35	PRO	-	expression tag	UNP Q85365
E	36	LEU	-	expression tag	UNP Q85365
E	37	GLY	-	expression tag	UNP Q85365
E	38	SER	-	expression tag	UNP Q85365
G	34	GLY	-	expression tag	UNP Q85365
G	35	PRO	-	expression tag	UNP Q85365

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Chain	Residue	Modelled	Actual	Comment	Reference
G	36	LEU	-	expression tag	UNP Q85365
G	37	GLY	-	expression tag	UNP Q85365
G	38	SER	-	expression tag	UNP Q85365
I	34	GLY	-	expression tag	UNP Q85365
I	35	PRO	-	expression tag	UNP Q85365
I	36	LEU	-	expression tag	UNP Q85365
I	37	GLY	-	expression tag	UNP Q85365
I	38	SER	-	expression tag	UNP Q85365
K	34	GLY	-	expression tag	UNP Q85365
K	35	PRO	-	expression tag	UNP Q85365
K	36	LEU	-	expression tag	UNP Q85365
K	37	GLY	-	expression tag	UNP Q85365
K	38	SER	-	expression tag	UNP Q85365

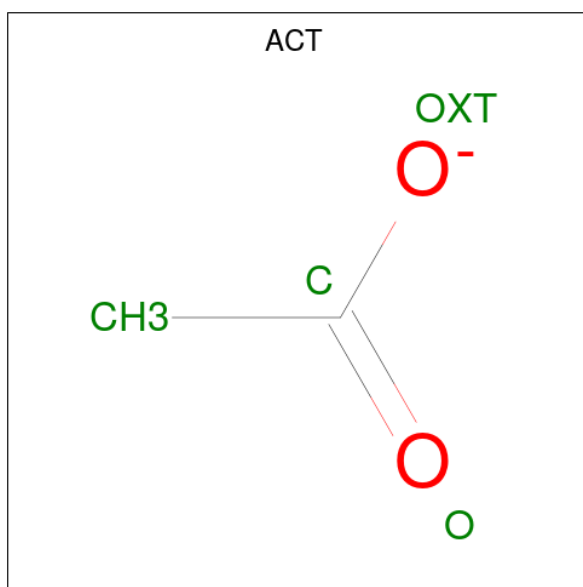
- Molecule 2 is a protein called BCL-2 HOMOLOGOUS ANTAGONIST/KILLER.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	23	Total	C	H	N	O	S	0	1	0
			360	111	174	38	36	1			
2	D	23	Total	C	H	N	O	S	0	0	0
			341	100	170	35	35	1			
2	F	23	Total	C	H	N	O	S	0	0	0
			352	106	174	35	36	1			
2	H	23	Total	C	H	N	O	S	0	0	0
			352	106	174	35	36	1			
2	J	24	Total	C	H	N	O	S	0	0	0
			363	109	179	36	38	1			
2	L	22	Total	C	H	N	O	S	0	0	0
			341	103	169	34	34	1			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			7	2	3	2		
4	E	1	Total	C	H	O	0	0
			7	2	3	2		
4	G	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 5 is water.

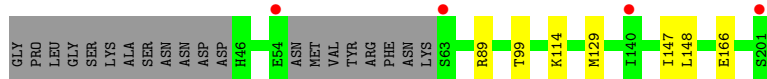
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	O	0	0
			30	30		
5	B	5	Total	O	0	0
			5	5		
5	C	17	Total	O	0	0
			17	17		
5	D	2	Total	O	0	0
			2	2		
5	E	10	Total	O	0	0
			10	10		
5	F	5	Total	O	0	0
			5	5		
5	G	12	Total	O	0	0
			12	12		
5	H	2	Total	O	0	0
			2	2		
5	I	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	3	Total 3	O 3	0	0
5	K	3	Total 3	O 3	0	0
5	L	2	Total 2	O 2	0	0

● Molecule 1: HOMOLOG OF VACCINIA VIRUS CDS F1L



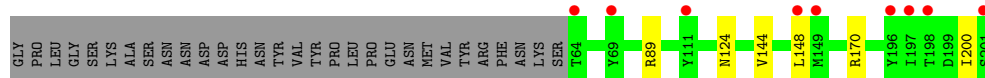
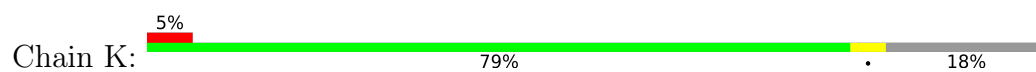
GLY	PRO	LEU	GLY	SER	LYS	ALA	SER	ASN	ASN	ASP	ASP	HIS	ASN	TYR	VAL	TYR	PRO	LEU	PRO	GLU	ASN	MET	VAL	TYR	ARG	PHE	ASN	ASN	LYS	S63	T147	S201
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GLY	PRO	LEU	GLY	SER	LYS	ALA	SER	ASN	ASN	ASP	ASP	HIS	N47	P51	LEU	PRO	PRO	GLU	ASN	MET	VAL	TYR	ARG	PHE	ASN	LYS	SER	THR	ASN	I66	L67	D68	M129	Y138	G168	T177	S201
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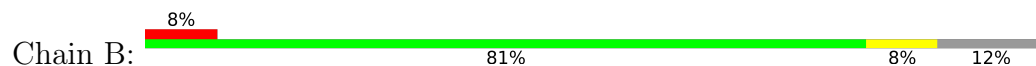
GLY	PRO	LEU	LEU	LYS	ALA	SER	ASN	ASP	ASP	HIS	ASN	TYR	VAL	TYR	PRO	LEU	PRO	GLU	ASN	MET	VAL	TYR	ARG	PHE	ASN	ASN	LYS	T64	N65	I66	T99	D118	T132	M149	I178	I200	SER
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GLY	PRO	LEU	GLY	SER	LYS	ALA	SER	ASN	ASN	ASP	ASP	HIS	ASN	TYR	VAL	PRO	PRO	GLU	ASN	MET	VAL	TYR	ARG	PHE	ASN	LYS	SER	THR	M65	I66	L67		M117		M123		S131		F135		I178		I194		I200		L201
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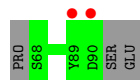
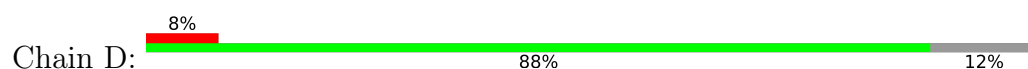




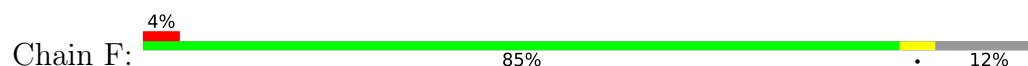
- Molecule 2: BCL-2 HOMOLOGOUS ANTAGONIST/KILLER



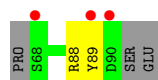
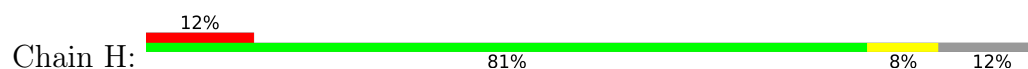
- Molecule 2: BCL-2 HOMOLOGOUS ANTAGONIST/KILLER



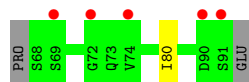
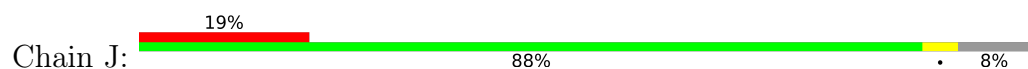
- Molecule 2: BCL-2 HOMOLOGOUS ANTAGONIST/KILLER



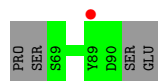
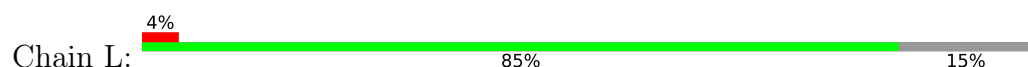
- Molecule 2: BCL-2 HOMOLOGOUS ANTAGONIST/KILLER



- Molecule 2: BCL-2 HOMOLOGOUS ANTAGONIST/KILLER



- Molecule 2: BCL-2 HOMOLOGOUS ANTAGONIST/KILLER



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.77Å 68.76Å 171.60Å 90.00° 109.43° 90.00°	Depositor
Resolution (Å)	39.70 – 2.55 39.70 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.70-2.55) 92.8 (39.70-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.197 , 0.240 0.203 , 0.246	Depositor DCC
R_{free} test set	2299 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15824	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CL

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	0.32	0/1231	0.62	0/1667
1	C	0.31	0/1151	0.60	0/1556
1	E	0.30	0/1178	0.61	0/1593
1	G	0.31	0/1139	0.62	0/1540
1	I	0.31	0/1138	0.62	0/1538
1	K	0.32	0/1145	0.63	0/1548
2	B	0.30	0/189	0.64	0/251
2	D	0.30	0/170	0.69	0/226
2	F	0.32	0/178	0.63	0/237
2	H	0.31	0/178	0.69	0/237
2	J	0.32	0/184	0.70	0/245
2	L	0.28	0/172	0.67	0/229
All	All	0.31	0/8053	0.62	0/10867

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1210	1176	1176	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1134	1110	1110	0	0
1	E	1159	1131	1131	3	0
1	G	1122	1100	1100	2	0
1	I	1121	1098	1098	2	0
1	K	1128	1105	1105	4	0
2	B	186	174	187	2	0
2	D	171	170	167	0	0
2	F	178	174	174	1	0
2	H	178	174	174	1	0
2	J	184	179	179	0	0
2	L	172	169	169	0	0
3	A	2	0	0	0	0
4	C	4	3	3	0	0
4	E	4	3	3	0	0
4	G	4	3	3	0	0
5	A	30	0	0	0	0
5	B	5	0	0	0	0
5	C	17	0	0	0	0
5	D	2	0	0	0	0
5	E	10	0	0	0	0
5	F	5	0	0	0	0
5	G	12	0	0	0	0
5	H	2	0	0	0	0
5	I	7	0	0	0	0
5	J	3	0	0	0	0
5	K	3	0	0	0	0
5	L	2	0	0	0	0
All	All	8055	7769	7779	10	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.

The worst 5 of 10 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:G:178:ILE:HG21	1:I:178:ILE:HG21	1.95	0.48
1:A:147:ILE:HD11	2:B:75:GLY:CA	2.44	0.47
1:G:118:ASP:OD2	2:H:88:ARG:NH2	2.48	0.47
1:E:177:THR:HG21	1:K:89:ARG:HD2	1.96	0.46
1:K:124:ASN:OD1	1:K:170:ARG:NH2	2.49	0.45

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	144/168 (86%)	141 (98%)	3 (2%)	0	100	100
1	C	137/168 (82%)	133 (97%)	4 (3%)	0	100	100
1	E	137/168 (82%)	135 (98%)	2 (2%)	0	100	100
1	G	135/168 (80%)	133 (98%)	2 (2%)	0	100	100
1	I	135/168 (80%)	133 (98%)	2 (2%)	0	100	100
1	K	136/168 (81%)	130 (96%)	6 (4%)	0	100	100
2	B	22/26 (85%)	22 (100%)	0	0	100	100
2	D	21/26 (81%)	21 (100%)	0	0	100	100
2	F	21/26 (81%)	21 (100%)	0	0	100	100
2	H	21/26 (81%)	21 (100%)	0	0	100	100
2	J	22/26 (85%)	22 (100%)	0	0	100	100
2	L	20/26 (77%)	20 (100%)	0	0	100	100
All	All	951/1164 (82%)	932 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	141/159 (89%)	136 (96%)	5 (4%)	32	48
1	C	133/159 (84%)	132 (99%)	1 (1%)	73	84
1	E	135/159 (85%)	132 (98%)	3 (2%)	45	64
1	G	131/159 (82%)	128 (98%)	3 (2%)	44	62
1	I	131/159 (82%)	129 (98%)	2 (2%)	57	74
1	K	132/159 (83%)	131 (99%)	1 (1%)	73	84
2	B	20/22 (91%)	20 (100%)	0	100	100
2	D	18/22 (82%)	18 (100%)	0	100	100
2	F	19/22 (86%)	19 (100%)	0	100	100
2	H	19/22 (86%)	18 (95%)	1 (5%)	20	31
2	J	20/22 (91%)	19 (95%)	1 (5%)	22	33
2	L	18/22 (82%)	18 (100%)	0	100	100
All	All	917/1086 (84%)	900 (98%)	17 (2%)	50	69

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	194	ILE
1	K	200	ILE
1	E	67	LEU
1	E	68	ASP
1	G	66	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	73	GLN
1	G	141	ASN
1	K	141	ASN
1	K	88	GLN
1	E	47	ASN

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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ACT	C	1202	-	3,3,3	0.83	0	3,3,3	1.35	0
4	ACT	G	1201	-	3,3,3	0.80	0	3,3,3	1.36	0
4	ACT	E	1202	-	3,3,3	0.81	0	3,3,3	1.29	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	148/168 (88%)	0.11	4 (2%) 56 57	41, 61, 106, 140	0
1	C	139/168 (82%)	0.05	1 (0%) 84 86	44, 63, 100, 121	0
1	E	141/168 (83%)	0.22	5 (3%) 47 48	46, 71, 116, 164	0
1	G	137/168 (81%)	0.04	1 (0%) 84 86	47, 69, 108, 145	0
1	I	137/168 (81%)	0.22	4 (2%) 53 55	51, 78, 141, 154	0
1	K	138/168 (82%)	0.36	9 (6%) 25 24	48, 84, 128, 169	0
2	B	23/26 (88%)	0.49	2 (8%) 16 15	41, 63, 121, 145	1 (4%)
2	D	23/26 (88%)	0.04	2 (8%) 16 15	53, 73, 103, 121	0
2	F	23/26 (88%)	0.34	1 (4%) 40 40	53, 64, 110, 136	0
2	H	23/26 (88%)	0.40	3 (13%) 7 6	53, 69, 122, 128	0
2	J	24/26 (92%)	1.10	5 (20%) 2 2	83, 99, 157, 173	0
2	L	22/26 (84%)	0.39	1 (4%) 38 38	70, 93, 128, 153	0
All	All	978/1164 (84%)	0.21	38 (3%) 43 44	41, 72, 126, 173	1 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	GLU	6.5
1	I	135	PHE	5.2
1	E	66	ILE	4.6
2	J	91	SER	4.1
1	K	201	SER	3.8

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	G	1201	4/4	0.45	0.23	76,77,91,91	1
4	ACT	C	1202	4/4	0.59	0.17	72,73,87,87	0
4	ACT	E	1202	4/4	0.65	0.23	71,71,86,86	0
3	CL	A	1202	1/1	0.83	0.19	83,83,83,83	0
3	CL	A	1203	1/1	0.88	0.11	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.