wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 01:45 PM EDT

PDB ID	:	6B4C
Title	:	Structure of Viperin from Trichoderma virens
Authors	:	Huang, R.H.; Selvadurai, K.
Deposited on	:	2017-09-26
Resolution	:	2.79 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 (i) 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 (i)) were used in the production of this report:

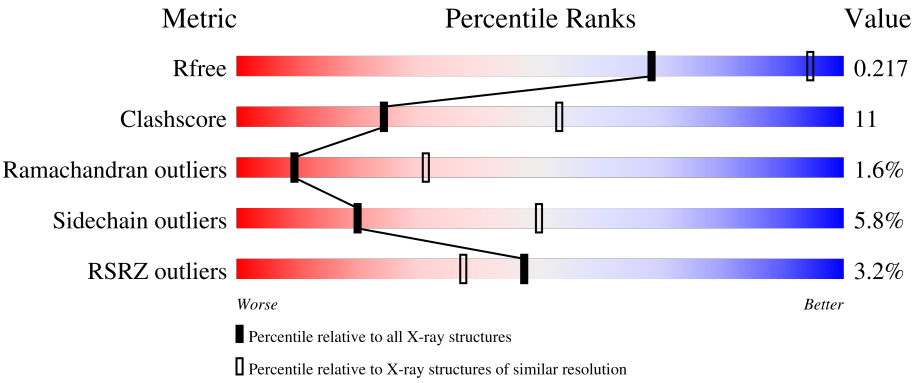
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	298	3% 69% 14% • • 13%
1	B	298	3% 65% 20% • 13%
1	C	298	2% 64% 20% • 13%
1	D	298	4% 68% 15% • • 12%
1	E	298	2% 66% 17% • • 14%

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Mol	Chain	Length	Quality of chain
1	F	298	3% 68% 17% 13%
1	G	298	3% 67% 16% 13%
1	H	298	2% 69% 15% 13%
1	I	298	2% 65% 19% 14%
1	J	298	3% 66% 17% 13%
1	K	298	4% 69% 17% 13%
1	L	298	2% 65% 17% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	402	-	-	X	-
2	SO4	G	402	-	-	X	-
2	SO4	J	401	-	-	X	-
2	SO4	K	402	-	-	X	-
3	FLC	A	403	-	-	X	-
3	FLC	B	403	-	-	X	-
3	FLC	C	403	-	-	X	-
3	FLC	D	403	-	-	X	-
3	FLC	E	403	-	-	X	-
3	FLC	G	403	-	-	X	-
3	FLC	H	403	-	-	X	-
3	FLC	I	403	-	X	X	-
3	FLC	K	403	-	X	X	-
3	FLC	L	403	-	-	X	-

2 Entry composition (i)

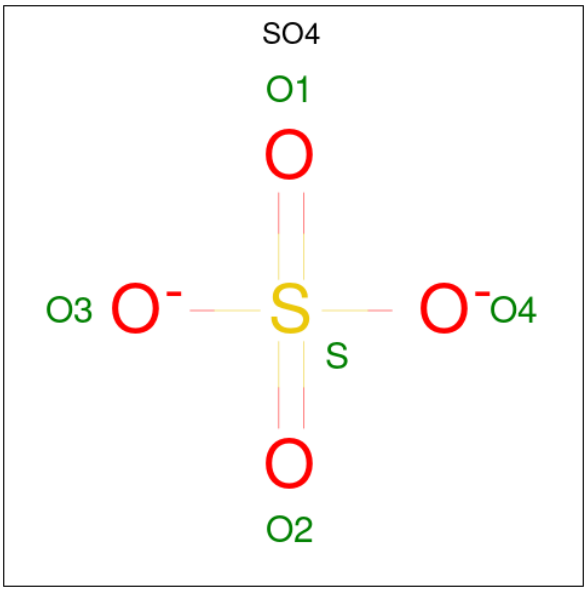
There are 4 unique types of molecules in this entry. The entry contains 25749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Viperin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2090	1329	363	387	11			
1	B	260	Total	C	N	O	S	0	0	0
			2083	1324	358	389	12			
1	C	260	Total	C	N	O	S	0	0	0
			2090	1329	361	388	12			
1	D	261	Total	C	N	O	S	0	0	0
			2093	1330	365	386	12			
1	E	256	Total	C	N	O	S	0	0	0
			2044	1303	350	379	12			
1	F	260	Total	C	N	O	S	0	0	0
			2078	1322	357	387	12			
1	G	259	Total	C	N	O	S	0	0	0
			2076	1321	359	385	11			
1	H	259	Total	C	N	O	S	0	0	0
			2073	1319	357	386	11			
1	I	257	Total	C	N	O	S	0	0	0
			2067	1316	357	382	12			
1	J	258	Total	C	N	O	S	0	0	0
			2075	1319	360	385	11			
1	K	260	Total	C	N	O	S	0	0	0
			2077	1324	357	385	11			
1	L	258	Total	C	N	O	S	0	0	0
			2066	1315	356	383	12			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0

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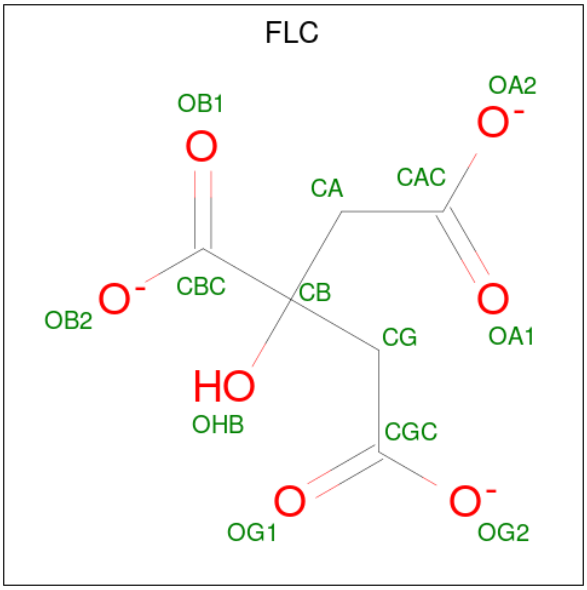
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	0	0
3	E	1	Total C O 13 6 7	0	0
3	F	1	Total C O 13 6 7	0	0
3	G	1	Total C O 13 6 7	0	0
3	H	1	Total C O 13 6 7	0	0
3	I	1	Total C O 13 6 7	0	0
3	J	1	Total C O 13 6 7	0	0
3	K	1	Total C O 13 6 7	0	0
3	L	1	Total C O 13 6 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	52	Total O 52 52	0	0
4	B	66	Total O 66 66	0	0
4	C	62	Total O 62 62	0	0
4	D	51	Total O 51 51	0	0
4	E	53	Total O 53 53	0	0
4	F	47	Total O 47 47	0	0
4	G	46	Total O 46 46	0	0
4	H	51	Total O 51 51	0	0

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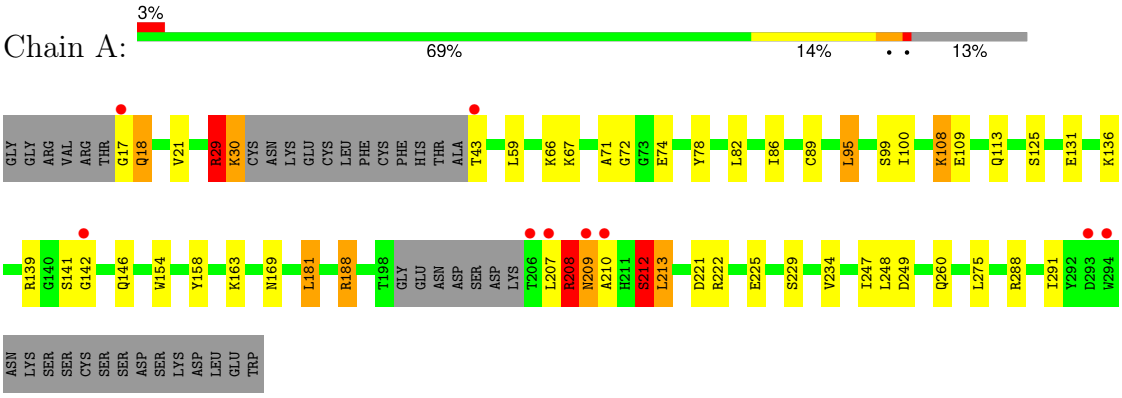
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	39	Total O 39 39	0	0
4	J	37	Total O 37 37	0	0
4	K	37	Total O 37 37	0	0
4	L	20	Total O 20 20	0	0

3 Residue-property plots (i)

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.

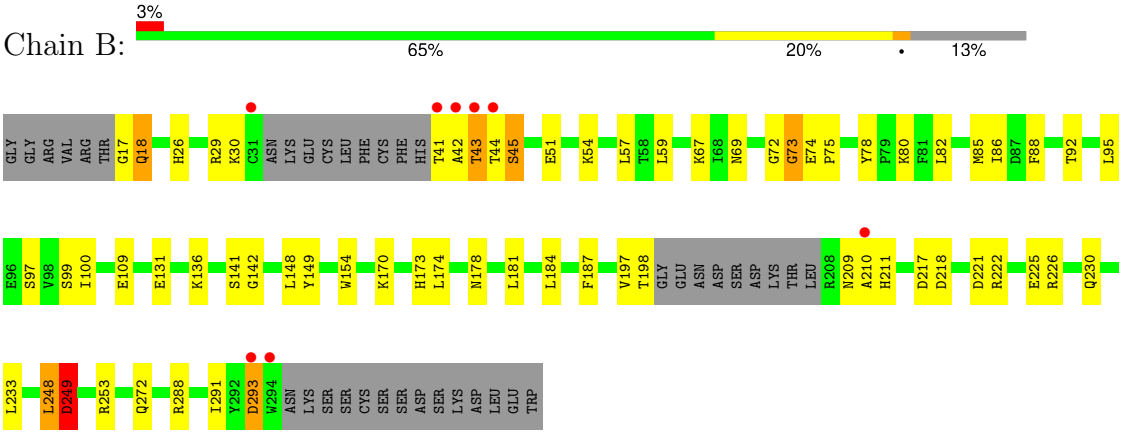
• Molecule 1: Viperin

Chain A:



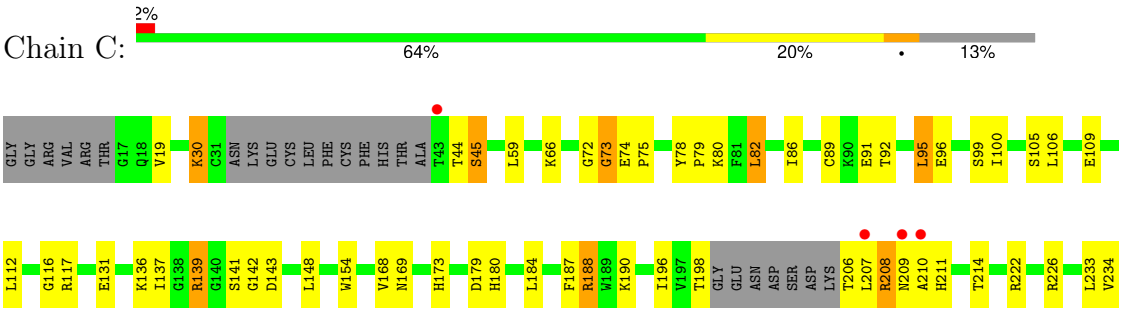
• Molecule 1: Viperin

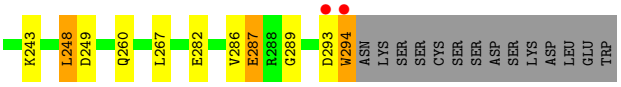
Chain B:



• Molecule 1: Viperin

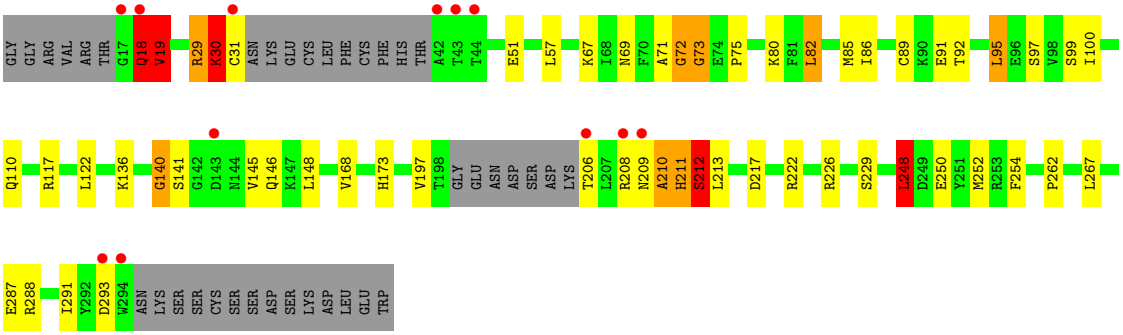
Chain C:





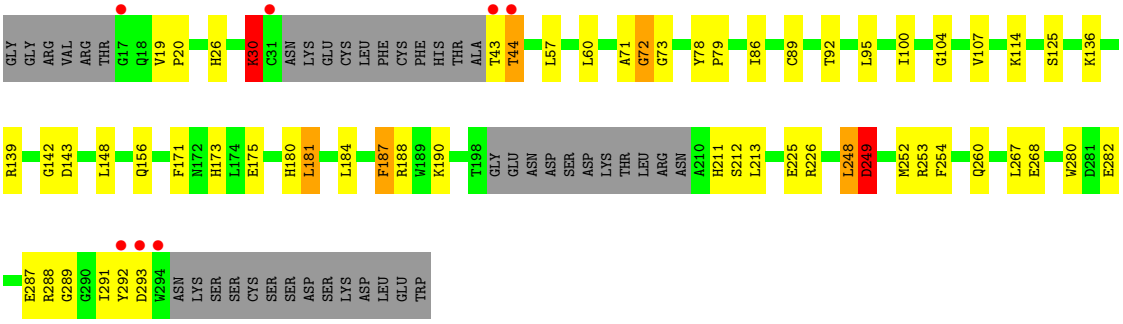
• Molecule 1: Viperin

Chain D:



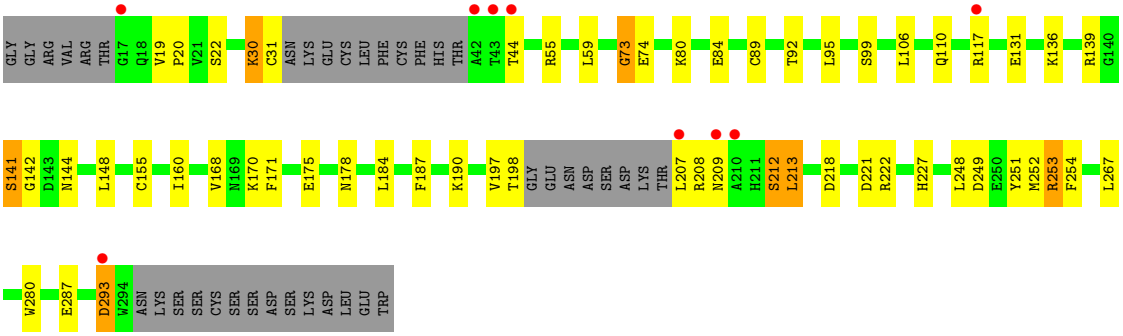
• Molecule 1: Viperin

Chain E:



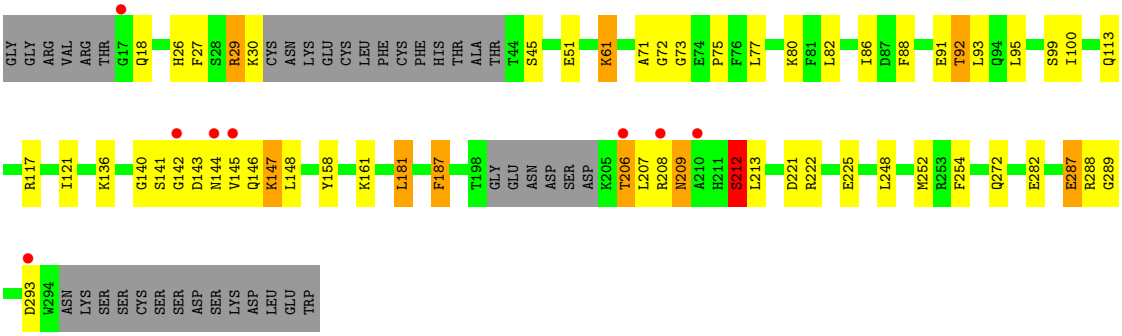
• Molecule 1: Viperin

Chain F:



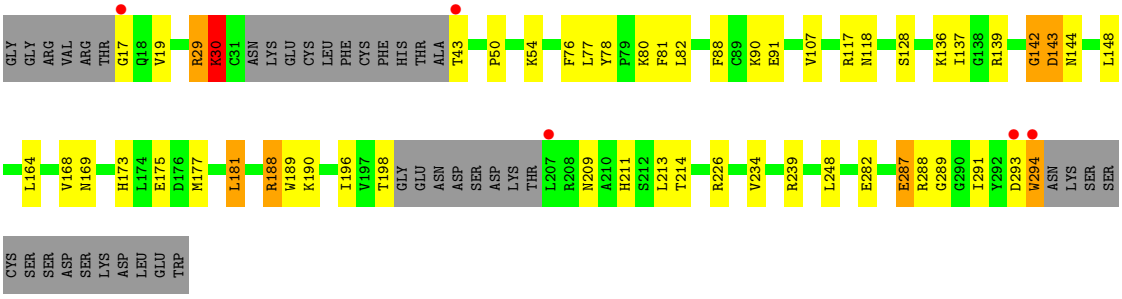
• Molecule 1: Viperin

Chain G:



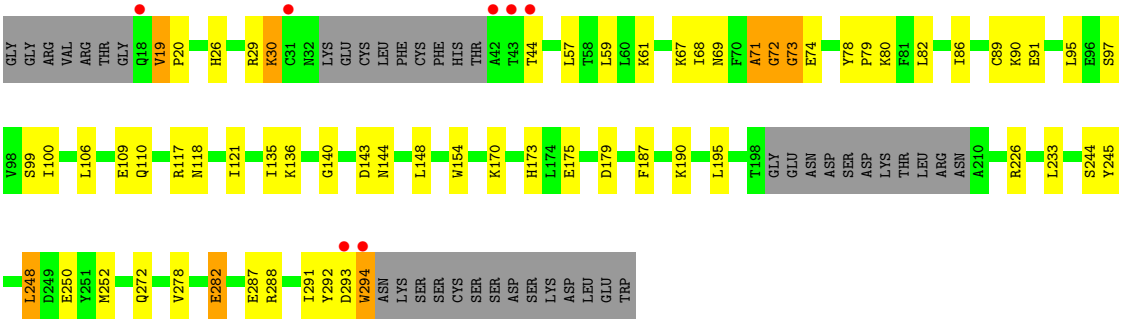
• Molecule 1: Viperin

Chain H:



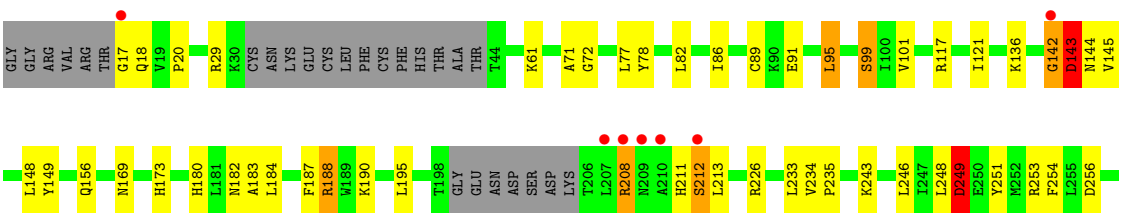
• Molecule 1: Viperin

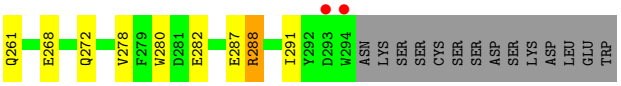
Chain I:



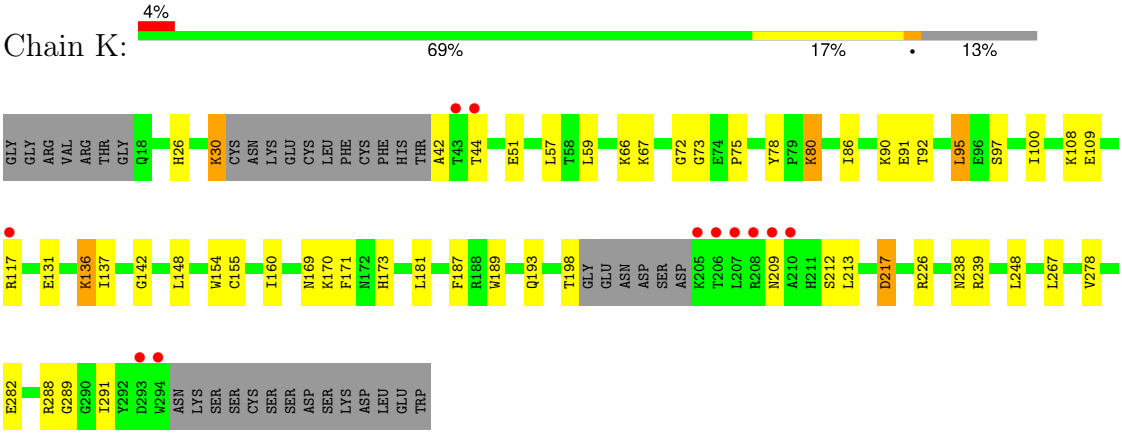
• Molecule 1: Viperin

Chain J:

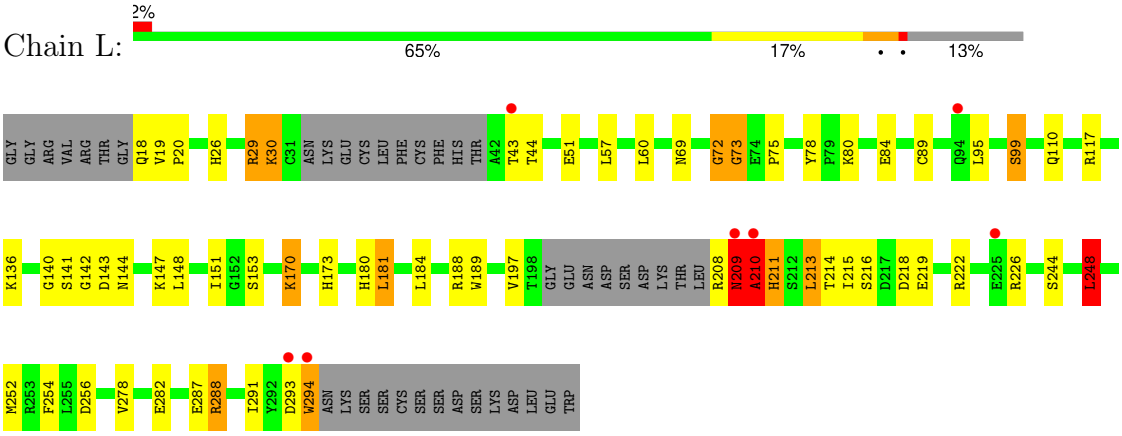




• Molecule 1: Viperin



• Molecule 1: Viperin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	173.88Å 209.57Å 233.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.81 – 2.79 49.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.81-2.79) 97.7 (49.85-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.85 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.190 , 0.211 0.195 , 0.217	Depositor DCC
R_{free} test set	2000 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25749	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FLC

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	0.92	7/2133 (0.3%)	0.79	5/2873 (0.2%)
1	B	0.68	0/2125	0.71	1/2864 (0.0%)
1	C	0.72	3/2133 (0.1%)	0.79	4/2874 (0.1%)
1	D	0.70	1/2136 (0.0%)	0.83	7/2877 (0.2%)
1	E	0.69	2/2086 (0.1%)	0.79	3/2811 (0.1%)
1	F	0.69	2/2121 (0.1%)	0.75	3/2859 (0.1%)
1	G	0.70	0/2119	0.79	5/2855 (0.2%)
1	H	0.71	3/2116 (0.1%)	0.74	4/2852 (0.1%)
1	I	0.67	1/2110 (0.0%)	0.71	1/2843 (0.0%)
1	J	0.70	1/2118 (0.0%)	0.84	5/2854 (0.2%)
1	K	0.68	2/2120 (0.1%)	0.73	2/2859 (0.1%)
1	L	0.71	3/2108 (0.1%)	0.78	3/2841 (0.1%)
All	All	0.72	25/25425 (0.1%)	0.77	43/34262 (0.1%)

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	D	0	2
1	E	0	2
1	F	0	2
1	G	0	1
1	H	0	1
1	I	0	2
1	J	0	1
1	L	0	4
All	All	0	15

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	LYS	CD-CE	15.11	1.89	1.51
1	A	108	LYS	CE-NZ	-15.08	1.11	1.49
1	A	30	LYS	CE-NZ	-13.67	1.14	1.49
1	F	117	ARG	CZ-NH1	-8.35	1.22	1.33
1	H	80	LYS	CD-CE	8.07	1.71	1.51

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	208	ARG	NE-CZ-NH2	-16.12	112.24	120.30
1	F	213	LEU	CA-CB-CG	10.29	138.96	115.30
1	G	72	GLY	N-CA-C	-9.97	88.18	113.10
1	E	73	GLY	N-CA-C	-9.83	88.53	113.10
1	E	72	GLY	N-CA-C	-9.69	88.88	113.10

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	210	ALA	Peptide
1	D	212	SER	Peptide
1	E	44	THR	Peptide
1	E	71	ALA	Peptide
1	F	139	ARG	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	2090	0	2053	44	0
1	B	2083	0	2042	43	0
1	C	2090	0	2047	65	0
1	D	2093	0	2047	41	0
1	E	2044	0	1997	40	0
1	F	2078	0	2026	37	0
1	G	2076	0	2022	44	0
1	H	2073	0	2017	38	0
1	I	2067	0	2028	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2075	0	2027	51	0
1	K	2077	0	2025	53	0
1	L	2066	0	2023	44	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	3	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	1	0
2	G	10	0	0	2	0
2	H	10	0	0	2	0
2	I	10	0	0	1	0
2	J	10	0	0	3	0
2	K	10	0	0	2	0
2	L	10	0	0	0	0
3	A	13	0	5	6	0
3	B	13	0	5	5	0
3	C	13	0	5	10	0
3	D	13	0	5	8	0
3	E	13	0	5	7	0
3	F	13	0	5	3	0
3	G	13	0	5	6	0
3	H	13	0	5	6	0
3	I	13	0	5	11	0
3	J	13	0	5	2	0
3	K	13	0	5	13	0
3	L	13	0	5	5	0
4	A	52	0	0	4	0
4	B	66	0	0	2	0
4	C	62	0	0	4	0
4	D	51	0	0	2	0
4	E	53	0	0	6	1
4	F	47	0	0	4	0
4	G	46	0	0	3	0
4	H	51	0	0	4	0
4	I	39	0	0	6	0
4	J	37	0	0	5	1
4	K	37	0	0	11	0
4	L	20	0	0	2	0
All	All	25749	0	24414	544	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 11.

The worst 5 of 544 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:108:LYS:CD	1:A:108:LYS:CE	1.89	1.51
1:I:288:ARG:HA	1:I:291:ILE:HD13	1.39	1.02
1:K:80:LYS:HE3	3:K:403:FLC:OHB	1.60	1.02
1:I:117:ARG:NH2	4:I:501:HOH:O	1.97	0.97
1:C:44:THR:HG22	1:C:45:SER:H	1.27	0.96

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)
4:E:549:HOH:O	4:J:526:HOH:O[3_554]	1.90	0.30

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	253/298 (85%)	231 (91%)	16 (6%)	6 (2%)	6 20
1	B	254/298 (85%)	238 (94%)	10 (4%)	6 (2%)	6 20
1	C	254/298 (85%)	239 (94%)	13 (5%)	2 (1%)	19 49
1	D	255/298 (86%)	241 (94%)	7 (3%)	7 (3%)	5 17
1	E	250/298 (84%)	239 (96%)	7 (3%)	4 (2%)	9 31
1	F	254/298 (85%)	242 (95%)	8 (3%)	4 (2%)	9 31
1	G	253/298 (85%)	237 (94%)	10 (4%)	6 (2%)	6 20
1	H	253/298 (85%)	236 (93%)	14 (6%)	3 (1%)	13 39
1	I	251/298 (84%)	239 (95%)	10 (4%)	2 (1%)	19 49
1	J	252/298 (85%)	231 (92%)	17 (7%)	4 (2%)	9 31
1	K	254/298 (85%)	239 (94%)	14 (6%)	1 (0%)	34 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	252/298 (85%)	233 (92%)	14 (6%)	5 (2%)	7 24
All	All	3035/3576 (85%)	2845 (94%)	140 (5%)	50 (2%)	9 31

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	B	43	THR
1	B	45	SER
1	B	210	ALA
1	B	249	ASP

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	230/267 (86%)	216 (94%)	14 (6%)	18 48
1	B	229/267 (86%)	214 (93%)	15 (7%)	16 44
1	C	230/267 (86%)	213 (93%)	17 (7%)	13 37
1	D	228/267 (85%)	214 (94%)	14 (6%)	18 48
1	E	223/267 (84%)	209 (94%)	14 (6%)	18 46
1	F	227/267 (85%)	210 (92%)	17 (8%)	13 37
1	G	226/267 (85%)	217 (96%)	9 (4%)	31 65
1	H	226/267 (85%)	218 (96%)	8 (4%)	36 70
1	I	227/267 (85%)	213 (94%)	14 (6%)	18 47
1	J	227/267 (85%)	212 (93%)	15 (7%)	16 44
1	K	226/267 (85%)	215 (95%)	11 (5%)	25 57
1	L	226/267 (85%)	216 (96%)	10 (4%)	28 61
All	All	2725/3204 (85%)	2567 (94%)	158 (6%)	20 50

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	143	ASP
1	K	187	PHE
1	I	248	LEU
1	J	188	ARG
1	L	117	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	178	ASN
1	L	118	ASN
1	G	182	ASN
1	L	26	HIS
1	G	144	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

36 ligands are modelled in this entry.

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	$\#\|Z\|>2$
2	SO4	D	402	-	4,4,4	0.41	0	6,6,6	0.26	0
3	FLC	F	403	-	12,12,12	1.27	2 (16%)	17,17,17	1.44	2 (11%)
2	SO4	G	401	-	4,4,4	0.35	0	6,6,6	0.28	0
2	SO4	L	401	-	4,4,4	0.28	0	6,6,6	0.54	0
3	FLC	C	403	-	12,12,12	1.76	3 (25%)	17,17,17	2.15	5 (29%)
3	FLC	L	403	-	12,12,12	1.28	1 (8%)	17,17,17	1.75	4 (23%)
2	SO4	I	401	-	4,4,4	0.32	0	6,6,6	0.25	0
2	SO4	A	401	-	4,4,4	0.31	0	6,6,6	0.28	0
2	SO4	K	402	-	4,4,4	0.20	0	6,6,6	0.43	0
3	FLC	D	403	-	12,12,12	1.85	4 (33%)	17,17,17	2.16	4 (23%)
3	FLC	H	403	-	12,12,12	3.11	4 (33%)	17,17,17	4.12	8 (47%)
2	SO4	J	402	-	4,4,4	0.34	0	6,6,6	0.33	0
2	SO4	E	402	-	4,4,4	0.40	0	6,6,6	0.21	0
2	SO4	K	401	-	4,4,4	0.26	0	6,6,6	0.18	0
3	FLC	J	403	-	12,12,12	1.34	2 (16%)	17,17,17	2.10	5 (29%)
2	SO4	C	401	-	4,4,4	0.22	0	6,6,6	0.32	0
2	SO4	B	402	-	4,4,4	0.51	0	6,6,6	0.54	0
2	SO4	H	402	-	4,4,4	0.41	0	6,6,6	0.38	0
2	SO4	G	402	-	4,4,4	0.31	0	6,6,6	0.30	0
2	SO4	E	401	-	4,4,4	0.28	0	6,6,6	0.51	0
2	SO4	I	402	-	4,4,4	0.37	0	6,6,6	0.25	0
3	FLC	E	403	-	12,12,12	1.80	2 (16%)	17,17,17	2.42	7 (41%)
3	FLC	K	403	-	12,12,12	2.58	4 (33%)	17,17,17	4.45	9 (52%)
2	SO4	D	401	-	4,4,4	0.33	0	6,6,6	0.74	0
2	SO4	F	402	-	4,4,4	0.43	0	6,6,6	0.57	0
2	SO4	A	402	-	4,4,4	0.48	0	6,6,6	0.34	0
3	FLC	G	403	-	12,12,12	1.49	3 (25%)	17,17,17	1.91	3 (17%)
3	FLC	I	403	-	12,12,12	4.02	4 (33%)	17,17,17	4.14	14 (82%)
2	SO4	B	401	-	4,4,4	0.25	0	6,6,6	0.21	0
2	SO4	C	402	-	4,4,4	0.27	0	6,6,6	0.61	0
2	SO4	F	401	-	4,4,4	0.37	0	6,6,6	0.31	0
2	SO4	J	401	-	4,4,4	0.31	0	6,6,6	0.29	0
3	FLC	A	403	-	12,12,12	1.67	3 (25%)	17,17,17	2.11	5 (29%)
2	SO4	H	401	-	4,4,4	0.42	0	6,6,6	0.56	0
2	SO4	L	402	-	4,4,4	0.34	0	6,6,6	0.31	0
3	FLC	B	403	-	12,12,12	1.34	1 (8%)	17,17,17	2.22	6 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	F	403	-	-	7/16/16/16	-
3	FLC	D	403	-	-	6/16/16/16	-
3	FLC	H	403	-	-	4/16/16/16	-
3	FLC	G	403	-	-	4/16/16/16	-
3	FLC	I	403	-	-	5/16/16/16	-
3	FLC	C	403	-	-	9/16/16/16	-
3	FLC	A	403	-	-	4/16/16/16	-
3	FLC	E	403	-	-	5/16/16/16	-
3	FLC	K	403	-	-	5/16/16/16	-
3	FLC	L	403	-	-	6/16/16/16	-
3	FLC	B	403	-	-	10/16/16/16	-
3	FLC	J	403	-	-	0/16/16/16	-

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	403	FLC	CB-CBC	12.51	1.66	1.53
3	H	403	FLC	CB-CBC	9.52	1.63	1.53
3	K	403	FLC	CB-CBC	7.52	1.61	1.53
3	D	403	FLC	CA-CB	-4.06	1.48	1.54
3	C	403	FLC	CB-CBC	3.86	1.57	1.53

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	403	FLC	OHB-CB-CBC	12.98	127.37	108.96
3	H	403	FLC	OHB-CB-CBC	12.55	126.76	108.96
3	K	403	FLC	OB2-CBC-CB	9.23	130.85	113.14
3	I	403	FLC	OHB-CB-CBC	6.50	118.17	108.96
3	I	403	FLC	OB2-CBC-CB	6.25	125.14	113.14

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	FLC	CG-CB-CBC-OB1
3	A	403	FLC	CG-CB-CBC-OB2
3	A	403	FLC	OHB-CB-CBC-OB1

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Mol	Chain	Res	Type	Atoms
3	A	403	FLC	OHB-CB-CBC-OB2
3	B	403	FLC	CG-CB-CBC-OB1

There are no ring outliers.

21 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	403	FLC	3	0
3	C	403	FLC	10	0
3	L	403	FLC	5	0
2	I	401	SO4	1	0
2	K	402	SO4	2	0
3	D	403	FLC	8	0
3	H	403	FLC	6	0
3	J	403	FLC	2	0
2	C	401	SO4	1	0
2	H	402	SO4	1	0
2	G	402	SO4	2	0
3	E	403	FLC	7	0
3	K	403	FLC	13	0
3	G	403	FLC	6	0
3	I	403	FLC	11	0
2	C	402	SO4	2	0
2	F	401	SO4	1	0
2	J	401	SO4	3	0
3	A	403	FLC	6	0
2	H	401	SO4	1	0
3	B	403	FLC	5	0

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, 95^{th} 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	259/298 (86%)	0.00	9 (3%)	44	34	27, 38, 72, 105	0
1	B	260/298 (87%)	0.01	8 (3%)	49	39	28, 38, 74, 92	0
1	C	260/298 (87%)	-0.03	6 (2%)	60	51	27, 39, 72, 95	0
1	D	261/298 (87%)	0.00	12 (4%)	32	22	28, 38, 72, 97	0
1	E	256/298 (85%)	-0.04	7 (2%)	54	44	29, 39, 68, 87	0
1	F	260/298 (87%)	0.09	9 (3%)	44	34	29, 42, 74, 94	0
1	G	259/298 (86%)	0.01	8 (3%)	49	39	28, 38, 67, 96	0
1	H	259/298 (86%)	-0.01	5 (1%)	66	59	30, 42, 70, 90	0
1	I	257/298 (86%)	0.01	7 (2%)	54	44	29, 42, 74, 90	0
1	J	258/298 (86%)	0.02	9 (3%)	44	34	33, 43, 71, 99	0
1	K	260/298 (87%)	0.08	11 (4%)	36	26	33, 44, 74, 101	0
1	L	258/298 (86%)	0.16	7 (2%)	54	44	34, 48, 72, 91	0
All	All	3107/3576 (86%)	0.03	98 (3%)	47	37	27, 41, 72, 105	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	294	TRP	6.7
1	A	43	THR	6.4
1	A	206	THR	5.7
1	F	210	ALA	5.5
1	G	17	GLY	5.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
3	FLC	K	403	13/13	0.79	0.35	47,56,74,83	0
3	FLC	I	403	13/13	0.81	0.38	45,56,72,72	0
3	FLC	L	403	13/13	0.83	0.29	53,59,69,72	0
3	FLC	D	403	13/13	0.85	0.28	43,50,64,66	0
3	FLC	C	403	13/13	0.86	0.28	41,51,64,66	0
3	FLC	B	403	13/13	0.86	0.30	41,54,63,71	0
3	FLC	F	403	13/13	0.86	0.31	45,52,64,68	0
3	FLC	E	403	13/13	0.87	0.29	45,50,61,61	0
3	FLC	G	403	13/13	0.88	0.27	43,48,59,61	0
3	FLC	J	403	13/13	0.88	0.26	49,55,63,66	0
3	FLC	A	403	13/13	0.89	0.31	44,51,61,63	0
3	FLC	H	403	13/13	0.89	0.29	46,59,74,74	0
2	SO4	B	402	5/5	0.91	0.24	59,63,86,88	0
2	SO4	F	402	5/5	0.91	0.25	66,67,87,90	0
2	SO4	L	402	5/5	0.91	0.35	73,79,96,100	0
2	SO4	I	402	5/5	0.92	0.20	65,74,84,94	0
2	SO4	K	402	5/5	0.93	0.25	66,66,77,83	0
2	SO4	H	402	5/5	0.93	0.21	61,69,72,82	0
2	SO4	A	402	5/5	0.94	0.25	64,65,75,84	0
2	SO4	G	402	5/5	0.94	0.29	66,68,83,91	0
2	SO4	E	402	5/5	0.94	0.27	63,66,80,84	0
2	SO4	C	402	5/5	0.95	0.23	65,65,83,85	0
2	SO4	H	401	5/5	0.95	0.13	55,61,63,68	0
2	SO4	D	402	5/5	0.96	0.26	62,66,81,83	0
2	SO4	J	402	5/5	0.96	0.24	71,72,85,88	0
2	SO4	I	401	5/5	0.97	0.13	56,59,66,67	0
2	SO4	L	401	5/5	0.97	0.11	62,64,70,77	0
2	SO4	G	401	5/5	0.97	0.10	58,60,68,68	0
2	SO4	D	401	5/5	0.97	0.13	49,56,62,63	0
2	SO4	K	401	5/5	0.97	0.12	51,59,66,70	0
2	SO4	E	401	5/5	0.98	0.09	53,54,65,65	0
2	SO4	C	401	5/5	0.98	0.10	53,55,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	J	401	5/5	0.98	0.09	57,59,70,78	0
2	SO4	F	401	5/5	0.98	0.10	57,61,64,70	0
2	SO4	B	401	5/5	0.98	0.10	60,62,67,67	0
2	SO4	A	401	5/5	0.99	0.10	51,57,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.