



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:33 PM UTC

PDB ID : 6VM6 / pdb_00006vm6
Title : Structure of *Acinetobacter baumannii* Cap4 SAVED/CARF-domain containing receptor with the cyclic trinucleotide 2'3'3'-cAAA
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Deposited on : 2020-01-27
Resolution : 2.10 Å (reported)

This is a Full wwPDB X-ray Structure Validation 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

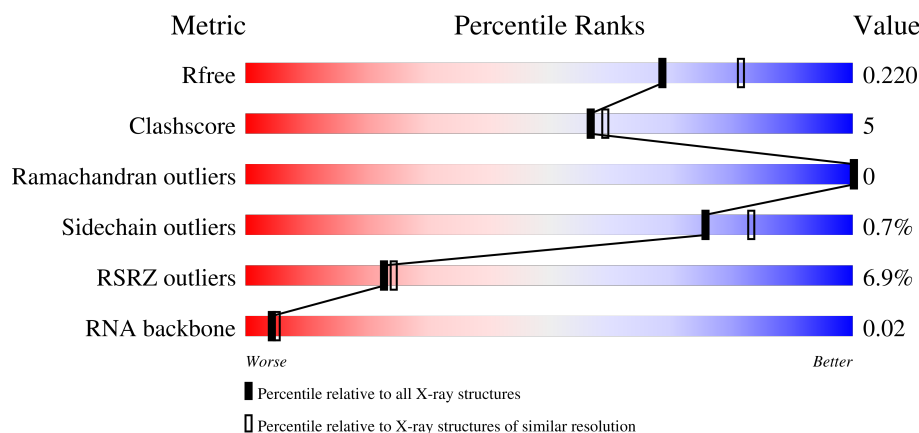
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)
RNA backbone	3983	1006 (2.42-1.78)

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	462	4% 86% 9% 5%
1	B	462	5% 85% 10% 5%
1	C	462	5% 88% 7% 5%

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Mol	Chain	Length	Quality of chain
1	D	462	
1	E	462	
1	F	462	
2	G	3	
2	H	3	
2	I	3	
2	J	3	
2	K	3	

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
3	SO4	B	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23004 atoms, of which 66 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 SAVED domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3518	2245	593	669	11			
1	B	440	Total	C	N	O	S	0	0	0
			3528	2250	595	672	11			
1	C	439	Total	C	N	O	S	0	0	0
			3522	2247	594	670	11			
1	D	440	Total	C	N	O	S	0	0	0
			3528	2250	595	672	11			
1	E	432	Total	C	N	O	S	0	0	0
			3472	2217	586	658	11			
1	F	437	Total	C	N	O	S	0	0	0
			3510	2239	592	668	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP C0VHC9
B	1	SER	-	expression tag	UNP C0VHC9
C	1	SER	-	expression tag	UNP C0VHC9
D	1	SER	-	expression tag	UNP C0VHC9
E	1	SER	-	expression tag	UNP C0VHC9
F	1	SER	-	expression tag	UNP C0VHC9

- Molecule 2 is a RNA chain called 2'-5'-Linked Cyclic RNA (5'-R(P*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	P	0	0	0
			66	30	15	18	3			
2	H	3	Total	C	H	N	O	P	0	0
			99	30	33	15	18	3		
2	I	3	Total	C	N	O	P	0	0	0
			66	30	15	18	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	3	Total	C	N	O	P	0	0	0
			66	30	15	18	3			
2	K	3	Total	C	H	N	O	P	0	0
			99	30	33	15	18	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

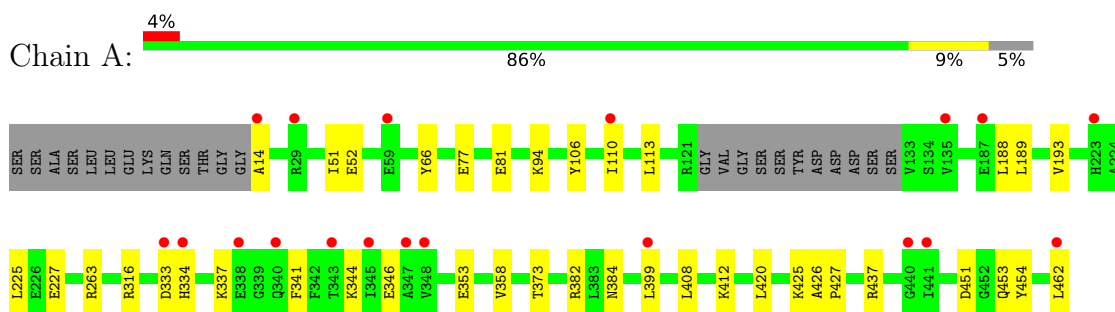
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	237	Total 237	O 237	0	0
4	B	277	Total 277	O 277	0	0
4	C	242	Total 242	O 242	0	0
4	D	272	Total 272	O 272	0	0
4	E	229	Total 229	O 229	0	0
4	F	220	Total 220	O 220	0	0
4	G	7	Total 7	O 7	0	0
4	H	3	Total 3	O 3	0	0
4	J	3	Total 3	O 3	0	0

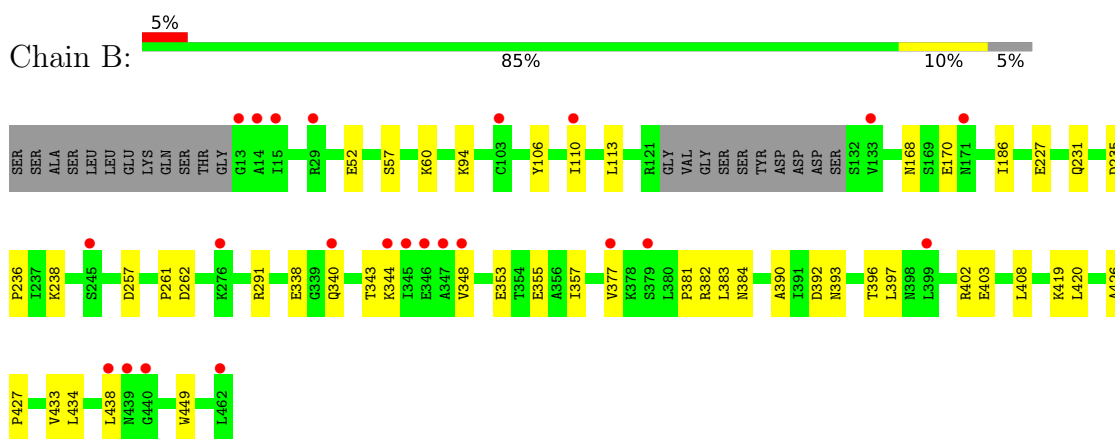
3 Residue-property plots [i](#)

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.

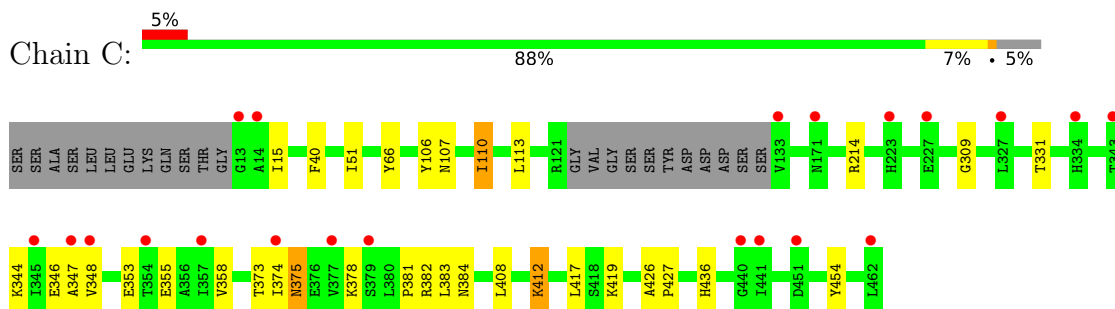
- Molecule 1: SAVED domain-containing protein



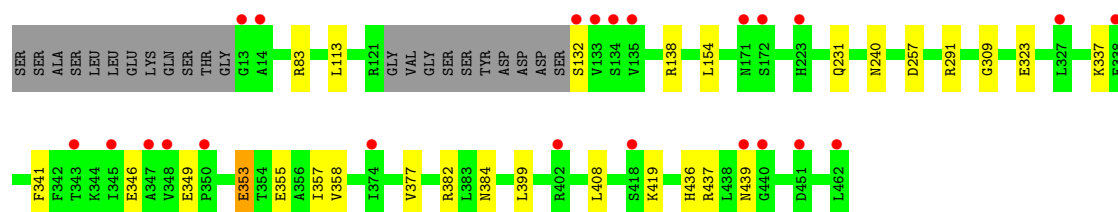
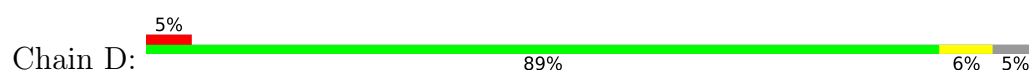
- Molecule 1: SAVED domain-containing protein



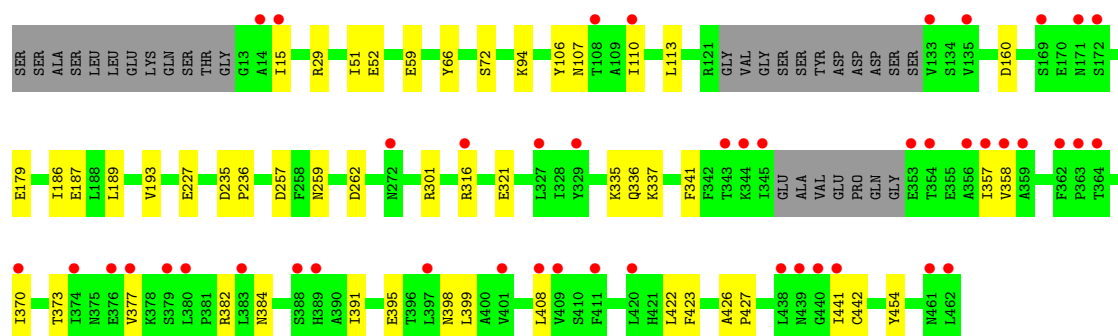
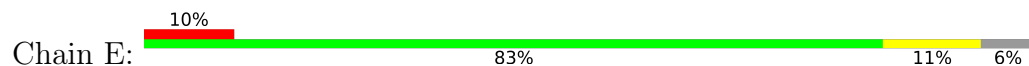
- Molecule 1: SAVED domain-containing protein



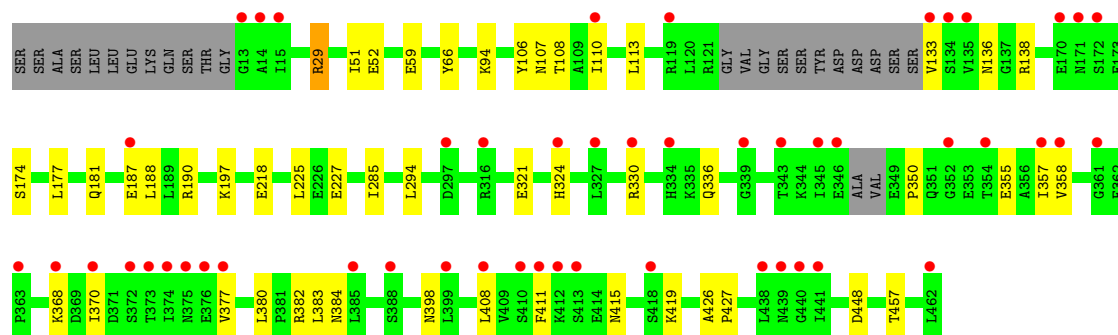
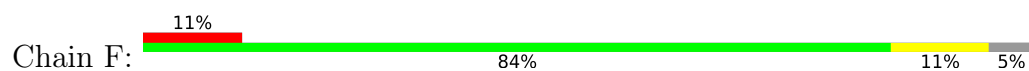
- Molecule 1: SAVED domain-containing protein



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- Molecule 1: SAVED domain-containing protein



- Molecule 2: 2'-5'-Linked Cyclic RNA (5'-R(P*AP*AP*A)-3')



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Chain I:  33% 67%

A1
A2
A3

- Molecule 2: 2'-5'-Linked Cyclic RNA (5'-R(P*AP*AP*A)-3')

Chain J:  67% 33%

A1
A2
A3

- Molecule 2: 2'-5'-Linked Cyclic RNA (5'-R(P*AP*AP*A)-3')

Chain K:  67% 33%

A1
A2
A3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.58Å 111.46Å 164.83Å 90.00° 100.21° 90.00°	Depositor
Resolution (Å)	49.21 – 2.10 49.21 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.21-2.10) 98.1 (49.21-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.185 , 0.219 0.188 , 0.220	Depositor DCC
R_{free} test set	2000 reflections (0.92%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23004	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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

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

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	0.13	0/3593	0.33	0/4856
1	B	0.15	0/3603	0.33	0/4869
1	C	0.14	0/3597	0.32	0/4861
1	D	0.15	0/3603	0.33	0/4869
1	E	0.15	0/3545	0.33	0/4788
1	F	0.14	0/3584	0.32	0/4841
2	G	3.51	12/74 (16.2%)	3.29	12/113 (10.6%)
2	H	3.51	10/74 (13.5%)	4.12	16/113 (14.2%)
2	I	3.70	14/74 (18.9%)	3.48	10/113 (8.8%)
2	J	3.65	13/74 (17.6%)	3.34	10/113 (8.8%)
2	K	3.57	11/74 (14.9%)	4.19	16/113 (14.2%)
All	All	0.49	60/21895 (0.3%)	0.61	64/29649 (0.2%)

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	3	A	C6-N6	10.14	1.54	1.33
2	H	3	A	C6-N6	9.90	1.53	1.33
2	I	3	A	C2'-O2'	9.63	1.56	1.42
2	J	3	A	C6-N6	9.57	1.53	1.33
2	J	3	A	C2'-O2'	9.54	1.56	1.42
2	I	3	A	C6-N6	9.52	1.52	1.33
2	G	3	A	C6-N6	9.41	1.52	1.33
2	K	2	A	N7-C5	8.91	1.57	1.39
2	H	2	A	N7-C5	8.69	1.56	1.39
2	G	3	A	C2'-O2'	8.66	1.55	1.42
2	K	3	A	C2'-O2'	8.57	1.54	1.41
2	G	2	A	N7-C5	8.49	1.56	1.39
2	K	2	A	C6-N6	8.46	1.50	1.33
2	J	2	A	N7-C5	8.44	1.56	1.39
2	I	2	A	N7-C5	8.44	1.56	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	3	A	C2'-O2'	8.31	1.54	1.41
2	H	2	A	C6-N6	8.25	1.50	1.33
2	K	1	A	C6-N6	8.03	1.50	1.33
2	H	1	A	C6-N6	7.97	1.50	1.33
2	G	1	A	C6-N6	7.83	1.49	1.33
2	J	1	A	C6-N6	7.81	1.49	1.33
2	I	1	A	C6-N6	7.75	1.49	1.33
2	J	2	A	C6-N6	7.60	1.49	1.33
2	G	2	A	C6-N6	7.54	1.49	1.33
2	I	2	A	C6-N6	7.53	1.49	1.33
2	I	3	A	C3'-O3'	6.90	1.52	1.42
2	I	1	A	P-O5'	6.80	1.70	1.59
2	J	1	A	P-O5'	6.72	1.69	1.59
2	G	2	A	O4'-C1'	5.99	1.50	1.42
2	K	1	A	P-O5'	5.97	1.68	1.59
2	I	2	A	O4'-C1'	5.86	1.50	1.42
2	H	3	A	N7-C5	5.84	1.50	1.39
2	J	2	A	O4'-C1'	5.84	1.50	1.42
2	K	1	A	O3'-P	5.81	1.69	1.61
2	G	1	A	O3'-P	5.80	1.69	1.61
2	G	1	A	N7-C5	5.78	1.50	1.39
2	I	3	A	O4'-C1'	5.78	1.50	1.41
2	K	1	A	N7-C5	5.75	1.50	1.39
2	I	1	A	N7-C5	5.73	1.50	1.39
2	J	1	A	N7-C5	5.71	1.50	1.39
2	G	1	A	P-O5'	5.68	1.68	1.59
2	J	3	A	O4'-C1'	5.68	1.50	1.41
2	J	3	A	C3'-C2'	5.66	1.61	1.52
2	H	1	A	N7-C5	5.66	1.50	1.39
2	J	3	A	C3'-O3'	5.64	1.50	1.42
2	H	1	A	O3'-P	5.61	1.69	1.61
2	I	1	A	O3'-P	5.59	1.69	1.61
2	K	1	A	O4'-C1'	5.48	1.49	1.41
2	G	3	A	N7-C5	5.48	1.50	1.39
2	I	3	A	P-O5'	5.43	1.67	1.59
2	I	3	A	N7-C5	5.37	1.50	1.39
2	K	3	A	P-O5'	5.35	1.67	1.59
2	J	1	A	O3'-P	5.32	1.69	1.61
2	J	3	A	N7-C5	5.31	1.49	1.39
2	K	3	A	N7-C5	5.30	1.49	1.39
2	H	1	A	P-O5'	5.13	1.67	1.59
2	I	2	A	N9-C4	-5.09	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	3	A	P-O5'	5.07	1.67	1.59
2	G	3	A	P-O5'	5.06	1.67	1.59
2	G	2	A	N9-C4	-5.04	1.27	1.37

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	3	A	C1'-O4'-C4'	-15.38	94.32	109.70
2	H	3	A	O4'-C1'-C2'	15.31	121.11	105.80
2	H	3	A	C1'-O4'-C4'	-15.24	94.46	109.70
2	K	3	A	O4'-C1'-C2'	15.15	120.95	105.80
2	I	3	A	C5'-C4'-C3'	-14.76	93.85	116.00
2	K	3	A	C3'-C2'-O2'	13.90	135.45	114.60
2	H	3	A	C3'-C2'-O2'	13.57	134.95	114.60
2	J	3	A	C5'-C4'-C3'	-13.27	96.10	116.00
2	K	3	A	O4'-C4'-C3'	13.16	119.26	106.10
2	G	3	A	C3'-C2'-O2'	12.46	129.39	110.70
2	H	3	A	O4'-C4'-C3'	12.28	118.38	106.10
2	I	2	A	O3'-P-O5'	10.11	119.16	104.00
2	I	3	A	C3'-C2'-O2'	9.87	125.50	110.70
2	H	2	A	O3'-P-O5'	9.75	118.62	104.00
2	I	1	A	O3'-P-O5'	9.72	118.58	104.00
2	K	2	A	O3'-P-O5'	9.70	118.55	104.00
2	J	2	A	O3'-P-O5'	9.59	118.39	104.00
2	G	1	A	O3'-P-O5'	9.34	118.01	104.00
2	G	2	A	O3'-P-O5'	9.29	117.94	104.00
2	J	1	A	O3'-P-O5'	9.22	117.82	104.00
2	J	3	A	C3'-C2'-O2'	9.17	124.45	110.70
2	K	1	A	O3'-P-O5'	8.60	116.89	104.00
2	I	3	A	N9-C1'-C2'	-8.45	99.32	112.00
2	H	1	A	O3'-P-O5'	8.38	116.56	104.00
2	K	3	A	C1'-C2'-O2'	-8.28	99.38	111.80
2	G	3	A	O4'-C4'-C3'	8.24	112.24	104.00
2	K	2	A	C3'-C2'-O2'	-7.57	103.25	114.60
2	K	3	A	C4'-C3'-O3'	7.47	120.60	109.40
2	J	1	A	C3'-C2'-C1'	7.44	108.74	101.30
2	K	2	A	C8-N9-C4	7.41	128.02	105.80
2	H	2	A	C8-N9-C4	7.38	127.95	105.80
2	H	3	A	C1'-C2'-O2'	-7.35	100.77	111.80
2	I	1	A	C3'-C2'-C1'	7.35	108.65	101.30
2	G	3	A	C1'-O4'-C4'	-7.34	102.56	109.90
2	G	1	A	C3'-C2'-C1'	7.29	108.59	101.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	A	C3'-C2'-O2'	-7.26	103.71	114.60
2	J	3	A	O4'-C4'-C3'	7.25	111.25	104.00
2	I	2	A	C8-N9-C4	7.23	127.50	105.80
2	J	2	A	C8-N9-C4	7.21	127.42	105.80
2	H	2	A	C1'-C2'-O2'	7.17	122.56	111.80
2	G	2	A	C8-N9-C4	7.13	127.18	105.80
2	J	3	A	N9-C1'-C2'	-6.86	101.71	112.00
2	K	2	A	C1'-C2'-O2'	6.79	121.99	111.80
2	G	3	A	C5'-C4'-C3'	-6.71	105.93	116.00
2	I	3	A	O4'-C4'-C3'	6.64	110.64	104.00
2	H	3	A	C4'-C3'-C2'	6.38	108.98	102.60
2	H	3	A	C4'-C3'-O3'	6.34	118.91	109.40
2	K	1	A	C4'-C3'-C2'	6.32	108.92	102.60
2	J	1	A	O5'-C5'-C4'	-6.23	102.15	111.50
2	H	1	A	C3'-C2'-C1'	6.19	107.49	101.30
2	J	1	A	C1'-O4'-C4'	-6.17	103.73	109.90
2	K	3	A	C5'-C4'-C3'	-6.10	106.06	115.20
2	K	1	A	OP1-P-OP2	-5.76	102.33	119.60
2	I	1	A	C1'-O4'-C4'	-5.73	104.17	109.90
2	K	1	A	C3'-C2'-C1'	5.69	106.99	101.30
2	G	1	A	C1'-O4'-C4'	-5.52	104.38	109.90
2	G	3	A	O4'-C1'-C2'	5.52	113.12	107.60
2	H	3	A	C5'-C4'-C3'	-5.51	106.94	115.20
2	G	3	A	C4'-C3'-C2'	5.50	108.10	102.60
2	H	1	A	C4'-C3'-C2'	5.34	107.94	102.60
2	G	1	A	C2'-C3'-O3'	-5.33	105.71	113.70
2	H	3	A	C3'-C2'-C1'	-5.24	96.26	101.50
2	K	3	A	C4'-C3'-C2'	5.15	107.75	102.60
2	I	1	A	O4'-C4'-C3'	5.10	109.10	104.00

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	3518	0	3466	30	0
1	B	3528	0	3474	29	0
1	C	3522	0	3469	23	0
1	D	3528	0	3474	22	0
1	E	3472	0	3424	48	0
1	F	3510	0	3454	38	0
2	G	66	0	33	0	0
2	H	66	33	33	1	0
2	I	66	0	33	3	0
2	J	66	0	33	1	0
2	K	66	33	33	13	0
3	A	5	0	0	0	0
3	B	5	0	0	3	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	10	0	0	0	0
4	A	237	0	0	11	0
4	B	277	0	0	13	0
4	C	242	0	0	2	0
4	D	272	0	0	10	0
4	E	229	0	0	11	0
4	F	220	0	0	14	0
4	G	7	0	0	0	0
4	H	3	0	0	0	0
4	J	3	0	0	0	0
All	All	22938	66	20926	193	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 5.

All (193) 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:E:160:ASP:OD1	4:E:601:HOH:O	1.83	0.96
1:E:427:PRO:HB3	2:K:2:A:N7	1.82	0.95
1:B:343:THR:OG1	4:B:602:HOH:O	1.90	0.90
1:B:227:GLU:O	4:B:601:HOH:O	1.90	0.89
1:E:427:PRO:HB3	2:K:2:A:C5	2.09	0.87
1:F:136:ASN:ND2	4:F:601:HOH:O	2.05	0.86
1:F:133:VAL:N	4:F:601:HOH:O	2.09	0.85
1:A:437:ARG:NH1	4:A:605:HOH:O	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ARG:NH1	4:D:604:HOH:O	2.14	0.81
1:E:427:PRO:HB3	2:K:2:A:C8	2.16	0.81
1:D:291:ARG:NH1	4:D:601:HOH:O	1.81	0.79
1:E:422:LEU:O	4:E:604:HOH:O	2.00	0.79
1:E:186:ILE:O	4:E:603:HOH:O	2.00	0.78
3:B:501:SO4:O4	4:B:603:HOH:O	2.04	0.76
1:E:262:ASP:OD2	1:F:108:THR:OG1	2.02	0.75
1:C:15:ILE:O	4:C:601:HOH:O	2.05	0.74
1:C:344:LYS:HE3	1:C:383:LEU:HD11	1.68	0.74
1:A:462:LEU:O	4:A:603:HOH:O	2.05	0.74
1:F:382:ARG:HH11	1:F:384:ASN:HD21	1.34	0.73
1:B:186:ILE:O	4:B:605:HOH:O	2.07	0.73
1:B:261:PRO:O	4:B:604:HOH:O	2.06	0.73
3:B:501:SO4:S	4:B:603:HOH:O	2.46	0.72
1:F:174:SER:O	4:F:603:HOH:O	2.08	0.72
1:F:138:ARG:NH1	4:F:606:HOH:O	2.23	0.70
1:A:454:TYR:O	4:A:604:HOH:O	2.08	0.70
1:B:238:LYS:HE3	4:B:694:HOH:O	1.91	0.70
1:B:449:TRP:O	4:B:606:HOH:O	2.10	0.70
1:D:231:GLN:OE1	4:D:602:HOH:O	2.11	0.67
1:A:453:GLN:HG2	4:A:622:HOH:O	1.95	0.66
1:F:133:VAL:CA	4:F:601:HOH:O	2.43	0.66
1:A:263:ARG:NH1	4:A:602:HOH:O	2.04	0.66
1:C:331:THR:OG1	4:C:602:HOH:O	2.13	0.65
1:C:348:VAL:HB	1:C:381:PRO:HA	1.77	0.65
1:A:344:LYS:HD2	4:A:618:HOH:O	1.97	0.65
1:A:451:ASP:OD2	4:A:606:HOH:O	2.14	0.65
1:F:357:ILE:HD11	1:F:377:VAL:O	1.98	0.63
1:E:259:ASN:HB3	2:K:1:A:C2	2.33	0.63
1:A:358:VAL:HG11	1:A:408:LEU:HD21	1.81	0.62
1:D:382:ARG:HH11	1:D:384:ASN:HD21	1.47	0.62
1:D:240:ASN:HB3	4:D:803:HOH:O	1.99	0.62
1:A:346:GLU:HG2	1:A:346:GLU:O	1.98	0.62
1:D:439:ASN:ND2	4:D:607:HOH:O	2.33	0.61
1:A:425:LYS:NZ	4:A:608:HOH:O	2.23	0.61
1:E:335:LYS:HE3	1:E:395:GLU:HB2	1.83	0.60
1:C:358:VAL:HG11	1:C:408:LEU:HD21	1.83	0.60
1:B:382:ARG:HH11	1:B:384:ASN:HD21	1.50	0.59
1:E:382:ARG:HH11	1:E:384:ASN:HD21	1.49	0.59
1:D:437:ARG:HD3	4:D:820:HOH:O	2.01	0.59
1:F:321:GLU:HG2	1:F:330:ARG:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:ARG:NH1	1:E:179:GLU:OE1	2.37	0.58
1:D:323:GLU:HB3	4:D:826:HOH:O	2.03	0.58
1:B:392:ASP:N	1:B:392:ASP:OD1	2.38	0.57
1:C:347:ALA:HB3	1:C:382:ARG:HB2	1.84	0.57
1:C:382:ARG:HE	1:C:384:ASN:HD21	1.53	0.57
1:E:59:GLU:OE2	4:E:605:HOH:O	2.17	0.57
1:A:337:LYS:O	1:A:399:LEU:HD12	2.05	0.56
1:B:52:GLU:OE1	1:B:94:LYS:NZ	2.36	0.56
1:C:382:ARG:NH1	1:C:384:ASN:OD1	2.38	0.56
1:E:106:TYR:HB3	1:E:110:ILE:HD11	1.86	0.56
1:F:187:GLU:HA	4:F:602:HOH:O	2.06	0.56
1:C:375:ASN:N	1:C:375:ASN:OD1	2.38	0.55
1:B:57:SER:HB3	1:B:60:LYS:O	2.06	0.55
1:F:59:GLU:HG3	4:F:610:HOH:O	2.07	0.55
1:D:357:ILE:HD11	1:D:377:VAL:O	2.06	0.55
1:F:218:GLU:OE1	4:F:604:HOH:O	2.18	0.55
1:F:357:ILE:HB	1:F:382:ARG:HA	1.89	0.55
1:A:341:PHE:HB2	1:A:399:LEU:HD22	1.88	0.54
1:D:337:LYS:O	1:D:399:LEU:HD12	2.08	0.54
1:E:59:GLU:HG3	4:E:605:HOH:O	2.08	0.53
1:C:358:VAL:HG22	1:C:383:LEU:HB3	1.91	0.53
3:B:501:SO4:O3	4:B:603:HOH:O	2.18	0.53
1:E:426:ALA:HB1	1:E:427:PRO:HD2	1.90	0.53
1:F:52:GLU:OE1	1:F:94:LYS:NZ	2.33	0.52
1:F:29:ARG:NE	4:F:608:HOH:O	2.32	0.52
2:I:3:A:N3	2:I:3:A:H2'	2.19	0.52
1:C:374:ILE:HD12	1:C:374:ILE:H	1.74	0.52
1:C:355:GLU:HG2	1:C:419:LYS:HB3	1.92	0.52
1:F:324:HIS:ND1	4:F:609:HOH:O	2.33	0.52
1:F:227:GLU:O	4:F:605:HOH:O	2.19	0.51
1:D:439:ASN:CB	4:D:607:HOH:O	2.58	0.51
1:B:355:GLU:HG2	1:B:419:LYS:HB3	1.91	0.51
1:F:368:LYS:HD2	1:F:368:LYS:H	1.76	0.51
1:E:358:VAL:HG11	1:E:408:LEU:HD21	1.92	0.51
1:D:341:PHE:HB2	1:D:399:LEU:HD22	1.92	0.51
1:D:83:ARG:HG3	1:D:154:LEU:HD11	1.93	0.50
1:C:51:ILE:HB	1:C:66:TYR:HB2	1.93	0.50
1:F:448:ASP:HB2	1:F:457:THR:HG21	1.93	0.50
1:B:231:GLN:OE1	4:B:607:HOH:O	2.20	0.50
1:C:426:ALA:HB1	1:C:427:PRO:HD2	1.94	0.50
1:B:168:ASN:HB3	1:B:170:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:LEU:HD21	1:F:197:LYS:HD3	1.93	0.50
1:F:382:ARG:NH1	1:F:384:ASN:HD21	2.05	0.50
1:F:357:ILE:HG13	1:F:380:LEU:HB2	1.93	0.49
1:F:29:ARG:NH1	4:F:613:HOH:O	2.44	0.49
1:C:375:ASN:HA	1:C:378:LYS:HG2	1.94	0.49
1:E:51:ILE:HB	1:E:66:TYR:HB2	1.94	0.49
1:E:321:GLU:OE1	4:E:606:HOH:O	2.20	0.49
1:A:51:ILE:HB	1:A:66:TYR:HB2	1.95	0.49
1:D:358:VAL:HG11	1:D:408:LEU:HD21	1.94	0.49
1:E:107:ASN:HB3	1:E:110:ILE:HG13	1.95	0.48
1:D:355:GLU:HG2	1:D:419:LYS:HB3	1.94	0.48
1:F:358:VAL:HG11	1:F:408:LEU:HD21	1.95	0.48
1:F:383:LEU:HD22	1:F:411:PHE:CG	2.49	0.48
1:D:346:GLU:HB3	1:D:349:GLU:OE1	2.13	0.48
1:E:257:ASP:OD2	1:F:107:ASN:ND2	2.46	0.48
1:D:439:ASN:HB2	4:D:607:HOH:O	2.14	0.47
1:C:373:THR:HG22	1:C:454:TYR:HB2	1.96	0.47
1:E:335:LYS:HG3	1:E:395:GLU:HG3	1.96	0.47
1:E:373:THR:HG22	1:E:454:TYR:HB2	1.94	0.47
1:B:340:GLN:HG3	1:B:403:GLU:OE2	2.14	0.47
1:F:426:ALA:HB1	1:F:427:PRO:HD2	1.96	0.47
2:I:2:A:H8	2:I:2:A:H2'	1.56	0.47
1:B:262:ASP:HA	4:B:604:HOH:O	2.14	0.47
1:C:106:TYR:HB3	1:C:110:ILE:HD11	1.96	0.47
1:F:51:ILE:HB	1:F:66:TYR:HB2	1.97	0.47
1:B:426:ALA:HB1	1:B:427:PRO:HD2	1.97	0.47
1:E:427:PRO:CB	2:K:2:A:C5	2.90	0.47
1:A:189:LEU:O	1:A:193:VAL:HG23	2.15	0.47
1:E:337:LYS:N	1:E:395:GLU:HG2	2.30	0.47
1:B:106:TYR:HB3	1:B:110:ILE:HD11	1.97	0.46
1:A:14:ALA:N	4:A:614:HOH:O	2.47	0.46
1:A:188:LEU:HD21	1:A:225:LEU:HD23	1.97	0.46
1:E:391:ILE:HB	2:K:2:A:N6	2.31	0.46
1:E:454:TYR:OH	2:K:3:A:N7	2.39	0.46
1:A:426:ALA:HB1	1:A:427:PRO:HD2	1.98	0.46
1:E:441:ILE:HG13	1:E:442:CYS:N	2.31	0.46
1:B:393:ASN:OD1	1:B:396:THR:N	2.39	0.46
1:D:257:ASP:OD2	1:E:107:ASN:ND2	2.49	0.46
1:F:181:GLN:NE2	4:F:602:HOH:O	2.49	0.45
1:E:357:ILE:HD11	1:E:377:VAL:O	2.16	0.45
2:J:3:A:N3	2:J:3:A:H2'	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:ILE:HB	2:K:2:A:H61	1.81	0.45
1:E:427:PRO:HB3	2:K:2:A:C4	2.50	0.45
1:F:188:LEU:HD21	1:F:225:LEU:HD23	1.98	0.45
1:A:106:TYR:HB3	1:A:110:ILE:HD11	1.99	0.45
1:C:353:GLU:HG3	1:C:381:PRO:CG	2.47	0.45
1:F:29:ARG:NH1	4:F:612:HOH:O	2.37	0.45
1:A:316:ARG:HD3	4:A:619:HOH:O	2.17	0.45
1:E:370:ILE:HD12	1:E:382:ARG:CZ	2.47	0.45
1:A:412:LYS:NZ	4:A:613:HOH:O	2.43	0.44
1:F:355:GLU:HG2	1:F:419:LYS:HB3	1.98	0.44
1:F:227:GLU:H	1:F:227:GLU:CD	2.25	0.44
1:B:402:ARG:NH2	4:B:617:HOH:O	2.50	0.44
1:E:301:ARG:HD3	2:K:1:A:O4'	2.18	0.44
1:E:337:LYS:O	1:E:399:LEU:HD12	2.17	0.44
1:A:52:GLU:OE1	1:A:94:LYS:NZ	2.41	0.44
1:F:350:PRO:HG2	1:F:415:ASN:OD1	2.18	0.44
1:A:333:ASP:O	1:A:334:HIS:HB2	2.18	0.44
1:F:370:ILE:HG13	1:F:382:ARG:CZ	2.47	0.44
1:A:382:ARG:HH11	1:A:384:ASN:HD21	1.65	0.43
1:B:348:VAL:HB	1:B:381:PRO:HA	2.00	0.43
1:C:412:LYS:HA	1:C:417:LEU:HD12	2.00	0.43
1:D:353:GLU:H	1:D:353:GLU:HG2	1.51	0.43
1:A:408:LEU:HD22	1:A:420:LEU:HD13	2.00	0.43
1:E:427:PRO:HG3	2:K:2:A:C6	2.53	0.43
1:B:291:ARG:NH1	4:B:614:HOH:O	2.45	0.43
1:E:316:ARG:HD3	4:E:618:HOH:O	2.19	0.43
1:E:341:PHE:HB2	1:E:399:LEU:HD22	2.01	0.43
1:A:337:LYS:C	1:A:399:LEU:HD12	2.43	0.43
1:E:427:PRO:HA	2:K:2:A:OP2	2.19	0.42
2:I:3:A:N3	2:I:3:A:H5'	2.34	0.42
1:E:423:PHE:HA	4:E:604:HOH:O	2.20	0.42
1:C:309:GLY:O	1:C:436:HIS:HA	2.19	0.42
1:B:408:LEU:HD22	1:B:420:LEU:HD13	2.02	0.42
1:A:358:VAL:HG21	1:A:408:LEU:CD2	2.50	0.42
1:E:189:LEU:O	1:E:193:VAL:HG23	2.19	0.42
1:B:344:LYS:HG3	1:B:383:LEU:HD11	2.02	0.42
1:F:285:ILE:HD13	1:F:294:LEU:HD21	2.01	0.42
1:E:52:GLU:OE1	1:E:94:LYS:NZ	2.43	0.41
1:B:434:LEU:O	1:B:438:LEU:HG	2.21	0.41
1:E:427:PRO:HD3	2:K:2:A:C4	2.55	0.41
1:B:397:LEU:HD21	1:B:433:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:SER:OG	4:E:602:HOH:O	1.92	0.41
1:E:262:ASP:HB2	4:E:637:HOH:O	2.20	0.41
1:A:227:GLU:H	1:A:227:GLU:CD	2.29	0.41
1:A:382:ARG:NE	1:A:384:ASN:OD1	2.54	0.41
1:B:357:ILE:HD11	1:B:377:VAL:O	2.21	0.41
1:E:15:ILE:HA	4:E:726:HOH:O	2.20	0.41
1:A:373:THR:HG22	1:A:454:TYR:HB2	2.01	0.41
1:B:257:ASP:OD2	1:C:107:ASN:ND2	2.53	0.41
1:B:390:ALA:HB1	2:H:2:A:N1	2.36	0.41
1:C:346:GLU:O	1:C:346:GLU:HG2	2.20	0.41
1:D:132:SER:N	4:D:626:HOH:O	2.54	0.41
1:F:336:GLN:HG2	1:F:398:ASN:HB3	2.03	0.41
1:E:235:ASP:HA	1:E:236:PRO:HD3	1.92	0.40
1:E:336:GLN:HG2	1:E:398:ASN:HB3	2.02	0.40
1:F:106:TYR:HB3	1:F:110:ILE:HD11	2.04	0.40
1:E:227:GLU:H	1:E:227:GLU:CD	2.29	0.40
1:A:77:GLU:O	1:A:81:GLU:HG2	2.22	0.40
1:B:235:ASP:HA	1:B:236:PRO:HD3	1.93	0.40
1:C:40:PHE:O	1:C:214:ARG:HD2	2.21	0.40
1:D:309:GLY:O	1:D:436:HIS:HA	2.21	0.40
1:D:337:LYS:C	1:D:399:LEU:HD12	2.47	0.40

There are no symmetry-related clashes.

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	434/462 (94%)	423 (98%)	11 (2%)	0	100	100
1	B	436/462 (94%)	427 (98%)	9 (2%)	0	100	100
1	C	435/462 (94%)	425 (98%)	10 (2%)	0	100	100
1	D	436/462 (94%)	429 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	426/462 (92%)	417 (98%)	9 (2%)	0	100	100
1	F	431/462 (93%)	421 (98%)	10 (2%)	0	100	100
All	All	2598/2772 (94%)	2542 (98%)	56 (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	392/411 (95%)	390 (100%)	2 (0%)	81	88
1	B	393/411 (96%)	390 (99%)	3 (1%)	73	81
1	C	392/411 (95%)	388 (99%)	4 (1%)	68	76
1	D	393/411 (96%)	391 (100%)	2 (0%)	81	88
1	E	387/411 (94%)	385 (100%)	2 (0%)	81	88
1	F	391/411 (95%)	388 (99%)	3 (1%)	73	81
All	All	2348/2466 (95%)	2332 (99%)	16 (1%)	76	83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	LEU
1	A	353	GLU
1	B	113	LEU
1	B	338	GLU
1	B	353	GLU
1	C	110	ILE
1	C	113	LEU
1	C	375	ASN
1	C	412	LYS
1	D	113	LEU
1	D	353	GLU
1	E	113	LEU

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Mol	Chain	Res	Type
1	E	187	GLU
1	F	29	ARG
1	F	113	LEU
1	F	190	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	B	252	ASN
1	B	415	ASN
1	B	439	ASN
1	C	219	ASN
1	C	223	HIS
1	D	181	GLN
1	D	336	GLN
1	D	375	ASN
1	E	168	ASN
1	E	181	GLN
1	E	219	ASN
1	E	324	HIS
1	E	439	ASN
1	F	181	GLN
1	F	202	ASN
1	F	265	GLN
1	F	384	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	3/3 (100%)	2 (66%)	1 (33%)
2	H	3/3 (100%)	2 (66%)	1 (33%)
2	I	3/3 (100%)	2 (66%)	1 (33%)
2	J	2/3 (66%)	1 (50%)	0
2	K	2/3 (66%)	1 (50%)	0
All	All	13/15 (86%)	8 (61%)	3 (23%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	2	A
2	G	3	A
2	H	2	A
2	H	3	A
2	I	2	A
2	I	3	A
2	J	3	A
2	K	3	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	G	1	A
2	H	1	A
2	I	1	A

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](#)

8 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	$\# Z > 2$
3	SO4	D	501	-	4,4,4	0.23	0	6,6,6	0.18	0
3	SO4	E	501	-	4,4,4	0.26	0	6,6,6	0.16	0
3	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	501	-	4,4,4	0.19	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.19	0
3	SO4	F	502	-	4,4,4	0.22	0	6,6,6	0.16	0
3	SO4	F	501	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	B	501	-	4,4,4	0.25	0	6,6,6	0.09	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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	SO4	3	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 [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	438/462 (94%)	0.25	19 (4%)	40	41	28, 47, 77, 101	0
1	B	440/462 (95%)	0.20	23 (5%)	33	35	25, 45, 85, 111	0
1	C	439/462 (95%)	0.36	21 (4%)	35	38	28, 49, 99, 130	0
1	D	440/462 (95%)	0.17	23 (5%)	33	35	28, 45, 82, 110	0
1	E	432/462 (93%)	0.48	46 (10%)	11	12	28, 53, 108, 129	0
1	F	437/462 (94%)	0.57	50 (11%)	10	10	31, 54, 114, 148	0
2	G	3/3 (100%)	-0.22	0	100	100	50, 50, 55, 56	0
2	H	3/3 (100%)	0.48	0	100	100	71, 71, 71, 74	0
2	I	3/3 (100%)	0.59	0	100	100	95, 95, 95, 97	0
2	J	3/3 (100%)	-0.14	0	100	100	46, 46, 52, 53	0
2	K	3/3 (100%)	1.23	0	100	100	81, 81, 81, 82	0
All	All	2641/2787 (94%)	0.34	182 (6%)	23	24	25, 49, 100, 148	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	ALA	6.3
1	E	345	ILE	5.4
1	B	171	ASN	5.1
1	E	441	ILE	5.1
1	C	13	GLY	4.7
1	C	374	ILE	4.7
1	E	462	LEU	4.5
1	F	374	ILE	4.5
1	D	13	GLY	4.4
1	B	103	CYS	4.3
1	E	438	LEU	4.2
1	F	133	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	347	ALA	4.2
1	E	133	VAL	4.2
1	C	345	ILE	4.1
1	E	14	ALA	4.0
1	C	348	VAL	4.0
1	A	14	ALA	3.9
1	D	462	LEU	3.9
1	F	462	LEU	3.9
1	C	440	GLY	3.8
1	F	327	LEU	3.8
1	D	14	ALA	3.7
1	C	133	VAL	3.7
1	E	374	ILE	3.7
1	C	354	THR	3.6
1	A	348	VAL	3.6
1	B	133	VAL	3.6
1	F	345	ILE	3.6
1	F	441	ILE	3.6
1	F	411	PHE	3.5
1	E	171	ASN	3.5
1	A	343	THR	3.5
1	F	377	VAL	3.5
1	D	374	ILE	3.4
1	A	440	GLY	3.4
1	D	348	VAL	3.4
1	C	14	ALA	3.4
1	F	13	GLY	3.4
1	D	133	VAL	3.3
1	A	347	ALA	3.3
1	B	462	LEU	3.2
1	F	14	ALA	3.2
1	C	462	LEU	3.2
1	D	347	ALA	3.1
1	F	15	ILE	3.1
1	E	172	SER	3.1
1	E	388	SER	3.1
1	D	343	THR	3.0
1	B	377	VAL	3.0
1	F	343	THR	3.0
1	F	354	THR	3.0
1	F	135	VAL	3.0
1	D	439	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	379	SER	2.9
1	F	358	VAL	2.9
1	F	370	ILE	2.9
1	D	350	PRO	2.9
1	E	327	LEU	2.9
1	E	440	GLY	2.9
1	C	377	VAL	2.9
1	F	363	PRO	2.9
1	C	343	THR	2.8
1	F	134	SER	2.8
1	E	343	THR	2.8
1	A	135	VAL	2.8
1	C	171	ASN	2.8
1	C	327	LEU	2.7
1	D	327	LEU	2.7
1	E	377	VAL	2.7
1	E	15	ILE	2.7
1	F	357	ILE	2.7
1	F	439	ASN	2.7
1	F	385	LEU	2.7
1	D	171	ASN	2.7
1	E	461	ASN	2.7
1	E	353	GLU	2.7
1	E	357	ILE	2.7
1	A	340	GLN	2.6
1	C	347	ALA	2.6
1	E	439	ASN	2.6
1	F	399	LEU	2.6
1	D	135	VAL	2.6
1	B	340	GLN	2.6
1	A	334	HIS	2.6
1	F	412	LYS	2.6
1	A	333	ASP	2.6
1	E	380	LEU	2.6
1	F	172	SER	2.6
1	F	418	SER	2.6
1	F	438	LEU	2.6
1	D	345	ILE	2.5
1	D	134	SER	2.5
1	E	363	PRO	2.5
1	A	462	LEU	2.5
1	E	397	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	135	VAL	2.5
1	F	372	SER	2.5
1	F	373	THR	2.5
1	C	441	ILE	2.5
1	B	346	GLU	2.4
1	B	344	LYS	2.4
1	A	223	HIS	2.4
1	C	334	HIS	2.4
1	F	324	HIS	2.4
1	D	440	GLY	2.4
1	B	15	ILE	2.4
1	B	245	SER	2.4
1	E	356	ALA	2.4
1	B	439	ASN	2.4
1	A	187	GLU	2.4
1	C	227	GLU	2.4
1	E	409	VAL	2.4
1	B	29	ARG	2.4
1	F	330	ARG	2.4
1	B	345	ILE	2.4
1	E	110	ILE	2.4
1	E	108	THR	2.4
1	B	276	LYS	2.3
1	F	170	GLU	2.3
1	E	408	LEU	2.3
1	F	368	LYS	2.3
1	D	418	SER	2.3
1	F	388	SER	2.3
1	A	29	ARG	2.3
1	E	383	LEU	2.3
1	F	408	LEU	2.3
1	A	338	GLU	2.3
1	B	379	SER	2.3
1	F	334	HIS	2.3
1	E	370	ILE	2.3
1	F	110	ILE	2.3
1	F	171	ASN	2.3
1	B	110	ILE	2.2
1	E	316	ARG	2.2
1	F	297	ASP	2.2
1	B	13	GLY	2.2
1	F	361	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	389	HIS	2.2
1	E	169	SER	2.2
1	E	379	SER	2.2
1	F	413	SER	2.2
1	A	110	ILE	2.2
1	F	440	GLY	2.2
1	E	420	LEU	2.2
1	F	375	ASN	2.2
1	E	354	THR	2.2
1	B	438	LEU	2.2
1	D	172	SER	2.2
1	E	411	PHE	2.1
1	E	401	VAL	2.1
1	F	352	GLY	2.1
1	F	316	ARG	2.1
1	F	376	GLU	2.1
1	A	441	ILE	2.1
1	D	223	HIS	2.1
1	E	358	VAL	2.1
1	B	399	LEU	2.1
1	F	410	SER	2.1
1	F	187	GLU	2.1
1	E	364	THR	2.1
1	B	440	GLY	2.1
1	C	357	ILE	2.1
1	F	119	ARG	2.1
1	E	359	ALA	2.1
1	D	451	ASP	2.1
1	A	345	ILE	2.1
1	B	348	VAL	2.1
1	E	362	PHE	2.1
1	A	59	GLU	2.0
1	D	132	SER	2.1
1	E	376	GLU	2.0
1	F	346	GLU	2.0
1	A	399	LEU	2.0
1	C	451	ASP	2.0
1	D	402	ARG	2.0
1	E	329	TYR	2.0
1	D	338	GLU	2.0
1	E	272	ASN	2.0
1	C	223	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	344	LYS	2.0
1	F	339	GLY	2.0

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(Å ²)	Q<0.9
3	SO4	C	502	5/5	0.67	0.15	128,128,129,131	0
3	SO4	F	501	5/5	0.67	0.19	134,134,136,136	0
3	SO4	D	501	5/5	0.94	0.10	46,52,58,66	0
3	SO4	A	501	5/5	0.94	0.09	49,55,60,62	0
3	SO4	E	501	5/5	0.95	0.10	41,49,56,63	0
3	SO4	C	501	5/5	0.95	0.11	48,51,60,66	0
3	SO4	B	501	5/5	0.96	0.10	47,48,54,64	0
3	SO4	F	502	5/5	0.96	0.08	50,52,60,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.