Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2023 – 08:26 am GMT

PDB ID	:	1UNJ
Title	:	Crystal structure of a 7-Aminoactinomycin D complex with non-complementary DNA
Authors	:	Alexopoulos, E.C.; Klement, R.; Jares-Erijman, E.A.; Uson, I.; Jovin, T.M.; Sheldrick, G.M.
Deposited on	:	2003-09-10
Resolution	:	2.50 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:

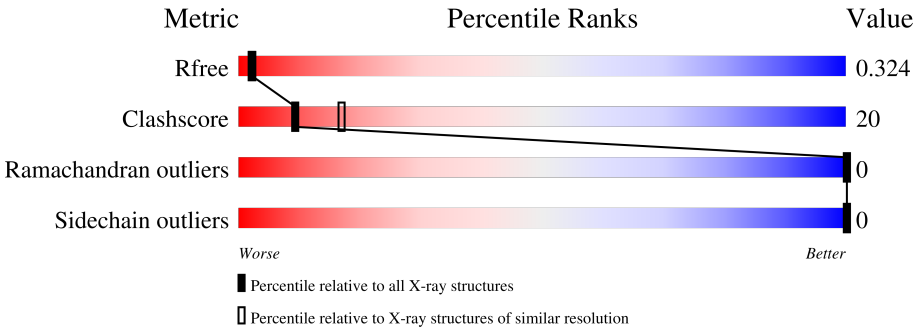
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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%

Mol	Chain	Length	Quality of chain
1	A	6	33% 50% 17%
1	B	6	33% 33% 33%
1	C	6	33% 33% 17% 17%
1	D	6	17% 67% 17%
1	G	6	33% 50% 17%
1	H	6	33% 33% 33%
1	I	6	17% 50% 17% 17%

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Mol	Chain	Length	Quality of chain
1	J	6	17% 67% 17%
1	M	6	50% 33% 17%
1	N	6	17% 67% 17%
1	O	6	17% 50% 17% 17%
1	P	6	17% 50% 17% 17%
1	S	6	83% 17%
1	T	6	50% 17% 17% 17%
1	U	6	67% 17% 17%
1	V	6	33% 67%
2	E	11	9% 73% 18%
2	F	11	55% 45%
2	K	11	36% 36% 27%
2	L	11	45% 55%
2	Q	11	27% 45% 27%
2	R	11	27% 64% 9%
2	W	11	36% 36% 27%
2	X	11	45% 36% 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2245 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 DNA chain called 5'-D(*TP*TP*AP*GP*BRU*TP)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	5	Total	Br	C	N	O	P	0	0	0
			103	1	49	16	32	5			
1	B	4	Total	Br	C	N	O	P	0	0	0
			82	1	39	14	24	4			
1	C	5	Total	Br	C	N	O	P	0	0	0
			87	1	39	14	28	5			
1	D	5	Total	Br	C	N	O	P	0	0	0
			103	1	49	16	32	5			
1	G	5	Total	Br	C	N	O	P	0	0	0
			99	1	49	16	29	4			
1	H	4	Total	Br	C	N	O	P	0	0	0
			82	1	39	14	24	4			
1	I	5	Total	Br	C	N	O	P	0	0	0
			86	1	39	14	27	5			
1	J	5	Total	Br	C	N	O	P	0	0	0
			99	1	49	16	29	4			
1	M	5	Total	Br	C	N	O	P	0	0	0
			103	1	49	16	32	5			
1	N	5	Total	Br	C	N	O	P	0	0	1
			84	1	39	14	26	4			
1	O	5	Total	Br	C	N	O	P	0	0	0
			86	1	39	14	27	5			
1	P	5	Total	Br	C	N	O	P	0	0	0
			103	1	49	16	32	5			
1	S	5	Total	Br	C	N	O	P	0	0	0
			103	1	49	16	32	5			
1	T	5	Total	Br	C	N	O	P	0	0	1
			83	1	39	14	25	4			
1	U	5	Total	Br	C	N	O	P	0	0	0
			82	1	39	14	24	4			
1	V	6	Total	Br	C	N	O	P	0	0	0
			118	1	58	18	36	5			

- Molecule 2 is a protein called 7-AMINO-ACTINOMYCIN D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	11	Total 91	C 62	N 13	O 16	0	0	0
2	F	11	Total 91	C 62	N 13	O 16	0	0	0
2	K	11	Total 91	C 62	N 13	O 16	0	0	0
2	L	11	Total 91	C 62	N 13	O 16	0	0	0
2	Q	11	Total 91	C 62	N 13	O 16	0	0	0
2	R	11	Total 91	C 62	N 13	O 16	0	0	0
2	W	11	Total 91	C 62	N 13	O 16	0	0	0
2	X	11	Total 91	C 62	N 13	O 16	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	6	PX1	PXZ	chromophore	NOR NOR00228
F	6	PX1	PXZ	chromophore	NOR NOR00228
K	6	PX1	PXZ	chromophore	NOR NOR00228
L	6	PX1	PXZ	chromophore	NOR NOR00228
Q	6	PX1	PXZ	chromophore	NOR NOR00228
R	6	PX1	PXZ	chromophore	NOR NOR00228
W	6	PX1	PXZ	chromophore	NOR NOR00228
X	6	PX1	PXZ	chromophore	NOR NOR00228

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	O 1	0	0
3	G	1	Total 1	O 1	0	0
3	I	1	Total 1	O 1	0	0
3	K	1	Total 1	O 1	0	0
3	L	2	Total 2	O 2	0	0

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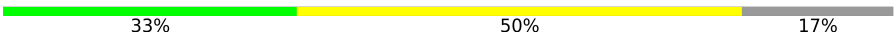
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	2	Total O 2 2	0	0
3	N	1	Total O 1 1	0	0
3	O	1	Total O 1 1	0	0
3	Q	1	Total O 1 1	0	0
3	R	1	Total O 1 1	0	0
3	S	1	Total O 1 1	0	0
3	W	1	Total O 1 1	0	0

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. 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. 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.

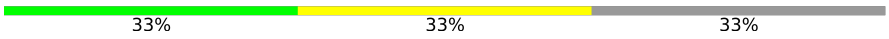
• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain A:



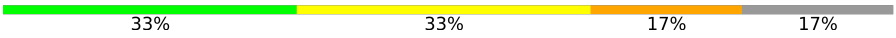
• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain B:



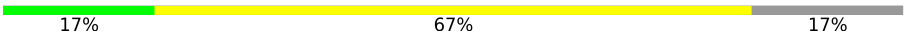
• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

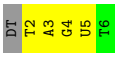
Chain C:



• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain D:



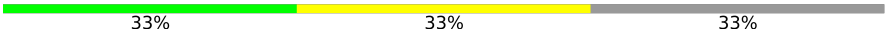


• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain G:

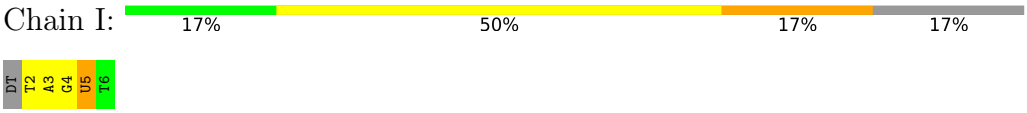
• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain H:



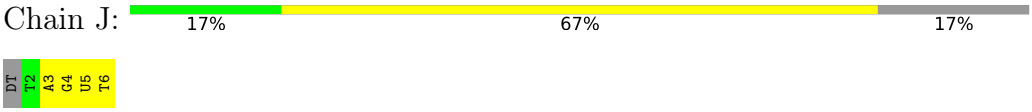
• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain I:



• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain J:

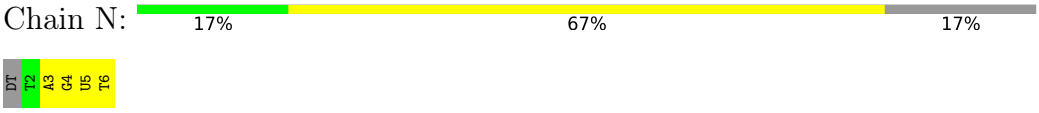


• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain M:

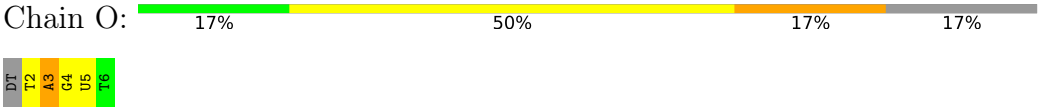
• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain N:



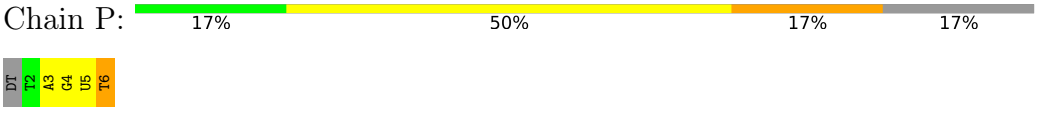
• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain O:



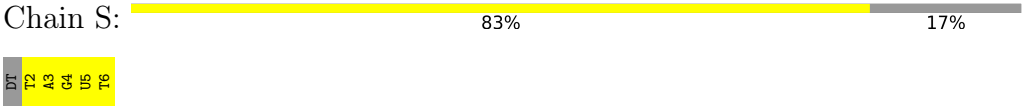
• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain P:



• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain S:



• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

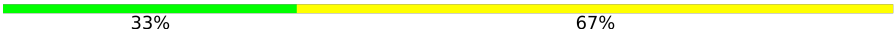
Chain T:

• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain U:

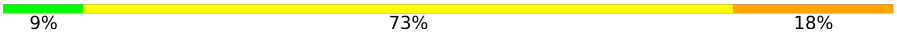
• Molecule 1: 5'-D(*TP*TP*AP*GP*BRU*TP)-3'

Chain V:



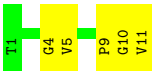
• Molecule 2: 7-AMINO-ACTINOMYCIN D

Chain E:



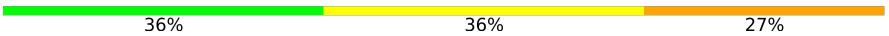
• Molecule 2: 7-AMINO-ACTINOMYCIN D

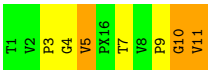
Chain F:



• Molecule 2: 7-AMINO-ACTINOMYCIN D

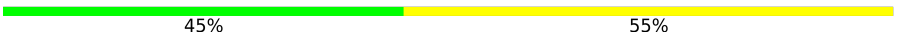
Chain K:

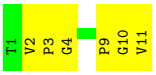




• Molecule 2: 7-AMINO-ACTINOMYCIN D

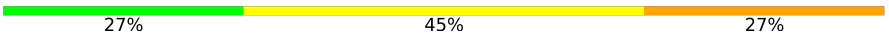
Chain L:

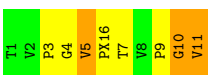




• Molecule 2: 7-AMINO-ACTINOMYCIN D

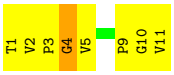
Chain Q:





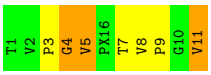
• Molecule 2: 7-AMINO-ACTINOMYCIN D

Chain R:



• Molecule 2: 7-AMINO-ACTINOMYCIN D

Chain W:



• Molecule 2: 7-AMINO-ACTINOMYCIN D

Chain X:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	71.22Å 71.22Å 108.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 22.79 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.50) 96.8 (22.79-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.33 (at 2.50Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.276 , 0.316 0.324 , 0.324	Depositor DCC
R_{free} test set	580 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	2245	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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 41.01 % 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 2.5160e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MVA, SAR, PX1, DVA, BRU

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	0.36	0/91	1.03	0/136
1	B	0.34	0/68	1.02	1/100 (1.0%)
1	C	0.42	0/73	0.98	1/109 (0.9%)
1	D	0.40	0/91	0.96	0/136
1	G	0.38	0/87	1.05	0/131
1	H	0.40	0/68	1.14	1/100 (1.0%)
1	I	0.37	0/72	0.85	0/107
1	J	0.41	0/87	0.95	0/131
1	M	0.40	0/91	1.06	0/136
1	N	0.41	0/70	1.14	1/105 (1.0%)
1	O	0.42	0/72	1.18	2/107 (1.9%)
1	P	0.42	0/91	1.13	1/136 (0.7%)
1	S	0.36	0/91	0.99	0/136
1	T	0.35	0/69	0.91	0/103
1	U	0.37	0/68	1.00	0/102
1	V	0.44	0/108	0.96	0/163
2	E	0.56	0/26	1.14	0/30
2	F	0.62	0/26	1.24	0/30
2	K	0.56	0/26	1.18	0/30
2	L	0.60	0/26	1.23	0/30
2	Q	0.63	0/26	1.19	0/30
2	R	0.59	0/26	1.19	0/30
2	W	0.59	0/26	1.08	0/30
2	X	0.60	0/26	1.24	0/30
All	All	0.43	0/1505	1.04	7/2178 (0.3%)

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
2	Q	0	1
2	R	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	3	DA	O4'-C1'-N9	-6.47	103.47	108.00
1	B	3	DA	O4'-C1'-N9	-6.22	103.64	108.00
1	P	6	DT	O4'-C4'-C3'	-6.19	102.02	104.50
1	H	3	DA	O4'-C1'-N9	-5.92	103.86	108.00
1	C	3	DA	O4'-C1'-N9	-5.44	104.19	108.00
1	O	3	DA	O4'-C1'-N9	-5.33	104.27	108.00
1	O	2	DT	O4'-C1'-N1	5.09	111.56	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Q	10	SAR	Mainchain
2	R	1	THR	Mainchain

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	103	0	56	2	0
1	B	82	0	42	0	0
1	C	87	0	43	2	0
1	D	103	0	56	2	0
1	G	99	0	54	3	0
1	H	82	0	42	0	0
1	I	86	0	43	3	1
1	J	99	0	54	2	1
1	M	103	0	56	2	0
1	N	84	0	44	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	86	0	43	3	0
1	P	103	0	56	2	0
1	S	103	0	56	7	0
1	T	83	0	42	3	0
1	U	82	0	41	0	0
1	V	118	0	65	3	0
2	E	91	0	84	10	0
2	F	91	0	84	5	0
2	K	91	0	82	8	0
2	L	91	0	84	6	0
2	Q	91	0	83	9	0
2	R	91	0	84	6	0
2	W	91	0	83	10	0
2	X	91	0	84	6	0
3	C	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	W	1	0	0	1	0
All	All	2245	0	1461	73	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 20.

All (73) 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:M:4:DG:H4'	2:Q:11:MVA:HG22	1.60	0.83
2:E:7:THR:O	2:E:9:PRO:HA	1.91	0.71
2:K:7:THR:O	2:K:9:PRO:HA	1.93	0.69
1:O:3:DA:N3	1:P:6:DT:H2'	2.08	0.67
1:M:4:DG:N3	2:Q:11:MVA:HN2	2.09	0.67
1:V:3:DA:H4'	1:V:4:DG:OP1	1.94	0.66
1:N:6:DT:H2"	1:S:3:DA:N6	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:6:DT:H5'	2:W:3:PRO:HG2	1.79	0.64
2:L:10:SAR:O	2:L:11:MVA:HG13	2.03	0.59
1:D:2:DT:C2	2:K:10:SAR:HN2	2.39	0.58
2:F:10:SAR:O	2:F:11:MVA:HG13	2.06	0.56
1:I:4:DG:N3	2:K:5:MVA:HN2	2.20	0.56
1:S:6:DT:H2'	1:T:3:DA:N3	2.20	0.55
2:E:1:THR:O	2:E:3:PRO:HA	2.06	0.55
2:R:10:SAR:O	2:R:11:MVA:HG13	2.07	0.54
2:W:7:THR:O	2:W:9:PRO:HA	2.08	0.54
2:E:3:PRO:HB3	2:E:6:PX1:O1'	2.09	0.53
2:F:9:PRO:HB2	1:G:2:DT:C2	2.43	0.53
1:N:6:DT:H2"	1:S:3:DA:H61	1.73	0.52
2:L:11:MVA:O	2:L:11:MVA:HG12	2.10	0.52
1:G:4:DG:H4'	2:K:11:MVA:HG22	1.90	0.52
2:K:5:MVA:HG12	2:K:5:MVA:O	2.10	0.51
1:N:4:DG:N3	2:R:5:MVA:HN2	2.26	0.51
2:X:11:MVA:O	2:X:11:MVA:HG12	2.09	0.51
2:W:4:SAR:O	2:W:5:MVA:HG13	2.11	0.50
2:K:4:SAR:O	2:K:5:MVA:HG13	2.12	0.50
1:O:4:DG:N3	2:Q:5:MVA:HN2	2.26	0.50
2:Q:11:MVA:HG23	2:Q:11:MVA:O	2.12	0.50
2:W:5:MVA:HG12	2:W:5:MVA:O	2.11	0.49
2:E:4:SAR:O	2:E:5:MVA:HG13	2.12	0.49
2:Q:7:THR:O	2:Q:9:PRO:HA	2.13	0.49
2:R:9:PRO:HB2	1:S:2:DT:C2	2.48	0.49
1:D:3:DA:H2"	1:D:4:DG:C4	2.48	0.49
1:S:6:DT:O4'	2:W:3:PRO:HB2	2.13	0.49
1:C:4:DG:N3	2:E:5:MVA:HN2	2.27	0.48
2:L:3:PRO:HA	2:L:4:SAR:HA3	1.56	0.48
1:G:4:DG:N3	2:K:11:MVA:HN2	2.28	0.48
1:J:3:DA:H2"	1:J:4:DG:C4	2.48	0.48
2:L:9:PRO:HA	2:L:10:SAR:HA3	1.43	0.47
1:I:3:DA:N3	1:J:6:DT:H2'	2.29	0.47
2:Q:4:SAR:O	2:Q:5:MVA:HG13	2.15	0.47
2:X:10:SAR:O	2:X:11:MVA:HG13	2.15	0.47
2:Q:3:PRO:HA	2:Q:4:SAR:HA3	1.63	0.47
1:A:4:DG:H4'	2:E:11:MVA:HG22	1.96	0.47
1:O:4:DG:H2"	2:Q:6:PX1:N2	2.30	0.47
2:F:9:PRO:HA	2:F:10:SAR:HA3	1.43	0.46
1:S:4:DG:H4'	2:W:11:MVA:HG22	1.98	0.46
2:K:3:PRO:HA	2:K:4:SAR:HA3	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:SAR:HN3	2:F:4:SAR:O	2.15	0.46
1:I:5:BRU:H2'	1:I:5:BRU:O2	2.15	0.46
2:X:2:DVA:HA	2:X:3:PRO:HA	1.83	0.46
1:T:5:BRU:BR	1:V:1:DT:C7	3.19	0.45
2:L:4:SAR:O	2:L:4:SAR:HN3	2.15	0.45
2:W:3:PRO:HA	2:W:4:SAR:HA3	1.62	0.45
2:X:4:SAR:O	2:X:4:SAR:HN3	2.17	0.45
2:R:9:PRO:HA	2:R:10:SAR:HA3	1.46	0.45
2:X:9:PRO:HA	2:X:10:SAR:HA3	1.57	0.44
2:E:3:PRO:HA	2:E:4:SAR:HA3	1.52	0.44
1:P:3:DA:H2"	1:P:4:DG:C4	2.53	0.43
2:R:4:SAR:HN3	2:R:4:SAR:O	2.18	0.43
2:W:3:PRO:HD2	3:W:2001:HOH:O	2.19	0.43
2:W:11:MVA:O	2:W:11:MVA:HG23	2.18	0.42
2:W:8:DVA:HA	2:W:9:PRO:HA	1.89	0.42
1:C:5:BRU:H2'	1:C:5:BRU:O2	2.18	0.42
2:X:3:PRO:HA	2:X:4:SAR:HA3	1.63	0.41
2:E:8:DVA:HA	2:E:9:PRO:HA	1.89	0.41
1:T:5:BRU:BR	1:V:1:DT:H73	2.75	0.41
2:Q:5:MVA:HG12	2:Q:5:MVA:O	2.20	0.41
2:E:2:DVA:O	2:E:2:DVA:HG12	2.21	0.41
2:R:2:DVA:HA	2:R:3:PRO:HA	1.84	0.41
2:L:2:DVA:HA	2:L:3:PRO:HA	1.82	0.40
2:E:5:MVA:O	2:E:5:MVA:HG12	2.20	0.40
1:A:6:DT:H2"	2:F:5:MVA:HG13	2.03	0.40

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)
1:I:2:DT:O4	1:J:3:DA:N6[4_466]	2.19	0.01

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	
2	E	2/11 (18%)	2 (100%)	0	0	100	100
2	F	2/11 (18%)	2 (100%)	0	0	100	100
2	K	2/11 (18%)	2 (100%)	0	0	100	100
2	L	2/11 (18%)	2 (100%)	0	0	100	100
2	Q	2/11 (18%)	2 (100%)	0	0	100	100
2	R	2/11 (18%)	2 (100%)	0	0	100	100
2	W	2/11 (18%)	2 (100%)	0	0	100	100
2	X	2/11 (18%)	2 (100%)	0	0	100	100
All	All	16/88 (18%)	16 (100%)	0	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	
2	E	4/4 (100%)	4 (100%)	0	100	100
2	F	4/4 (100%)	4 (100%)	0	100	100
2	K	4/4 (100%)	4 (100%)	0	100	100
2	L	4/4 (100%)	4 (100%)	0	100	100
2	Q	4/4 (100%)	4 (100%)	0	100	100
2	R	4/4 (100%)	4 (100%)	0	100	100
2	W	4/4 (100%)	4 (100%)	0	100	100
2	X	4/4 (100%)	4 (100%)	0	100	100
All	All	32/32 (100%)	32 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

64 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	BRU	B	5	1	18,21,22	0.47	0	26,30,33	0.95	1 (3%)
1	BRU	S	5	1	18,21,22	0.51	0	26,30,33	0.88	1 (3%)
2	MVA	R	11	2	6,7,8	0.37	0	7,8,10	0.93	0
1	BRU	V	5	1	18,21,22	0.53	0	26,30,33	0.90	1 (3%)
2	MVA	W	11	2	6,7,8	0.28	0	7,8,10	1.80	2 (28%)
2	MVA	K	11	2	6,7,8	0.37	0	7,8,10	1.51	1 (14%)
2	SAR	E	10	2	4,4,5	0.74	0	1,3,5	1.76	0
1	BRU	C	5	1	18,21,22	0.46	0	26,30,33	1.06	2 (7%)
2	MVA	X	11	2	6,7,8	0.43	0	7,8,10	1.09	1 (14%)
2	SAR	R	4	2	4,4,5	0.76	0	1,3,5	2.12	1 (100%)
2	SAR	K	4	2	4,4,5	0.72	0	1,3,5	1.80	0
2	SAR	X	4	2	4,4,5	0.73	0	1,3,5	2.04	1 (100%)
2	MVA	K	5	2	6,7,8	0.43	0	7,8,10	1.31	2 (28%)
2	MVA	X	5	2	6,7,8	0.75	0	7,8,10	0.66	0
2	MVA	Q	11	2	6,7,8	0.27	0	7,8,10	1.67	2 (28%)
1	BRU	G	5	1	18,21,22	0.46	0	26,30,33	0.83	1 (3%)
2	SAR	F	4	2	4,4,5	0.72	0	1,3,5	1.65	0
2	MVA	E	11	2	6,7,8	0.32	0	7,8,10	2.40	2 (28%)
1	BRU	P	5	1	18,21,22	0.48	0	26,30,33	0.88	1 (3%)
1	BRU	D	5	1	18,21,22	0.49	0	26,30,33	0.95	1 (3%)
1	BRU	O	5	1	18,21,22	0.52	0	26,30,33	1.09	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MVA	W	5	2	6,7,8	0.51	0	7,8,10	1.11	1 (14%)
2	SAR	Q	4	2	4,4,5	0.78	0	1,3,5	1.95	0
1	BRU	J	5	1	18,21,22	0.50	0	26,30,33	0.90	1 (3%)
2	SAR	E	4	2	4,4,5	0.71	0	1,3,5	1.97	0
1	BRU	N	5	1	18,21,22	0.45	0	26,30,33	0.98	2 (7%)
2	MVA	E	5	2	6,7,8	0.41	0	7,8,10	1.12	1 (14%)
2	SAR	W	4	2	4,4,5	0.74	0	1,3,5	2.05	1 (100%)
2	MVA	L	5	2	6,7,8	0.52	0	7,8,10	0.72	0
1	BRU	A	5	1	18,21,22	0.49	0	26,30,33	0.89	1 (3%)
2	MVA	L	11	2	6,7,8	0.43	0	7,8,10	0.78	0
2	SAR	W	10	2	4,4,5	0.75	0	1,3,5	1.92	0
2	MVA	Q	5	2	6,7,8	0.37	0	7,8,10	1.38	1 (14%)
1	BRU	I	5	1	18,21,22	0.54	0	26,30,33	1.04	1 (3%)
1	BRU	T	5	1	18,21,22	0.52	0	26,30,33	0.93	2 (7%)
2	SAR	X	10	2	4,4,5	0.77	0	1,3,5	1.86	0
2	MVA	R	5	2	6,7,8	0.48	0	7,8,10	0.50	0
2	SAR	F	10	2	4,4,5	0.76	0	1,3,5	1.74	0
2	SAR	Q	10	2	4,4,5	0.77	0	1,3,5	2.37	1 (100%)
2	MVA	F	11	2	6,7,8	0.53	0	7,8,10	0.72	0
1	BRU	U	5	1	18,21,22	0.52	0	26,30,33	0.91	2 (7%)
2	SAR	R	10	2	4,4,5	0.76	0	1,3,5	2.00	0
1	BRU	M	5	1	18,21,22	0.48	0	26,30,33	0.90	1 (3%)
2	SAR	L	4	2	4,4,5	0.71	0	1,3,5	1.67	0
2	SAR	L	10	2	4,4,5	0.71	0	1,3,5	1.58	0
2	MVA	F	5	2	6,7,8	0.53	0	7,8,10	0.95	0
2	SAR	K	10	2	4,4,5	0.76	0	1,3,5	2.08	1 (100%)
1	BRU	H	5	1	18,21,22	0.47	0	26,30,33	0.91	1 (3%)

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
1	BRU	B	5	1	-	2/7/21/22	0/2/2/2
1	BRU	S	5	1	-	0/7/21/22	0/2/2/2
2	MVA	R	11	2	-	3/6/8/10	-
1	BRU	V	5	1	-	3/7/21/22	0/2/2/2
2	MVA	W	11	2	-	1/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MVA	K	11	2	-	2/6/8/10	-
2	SAR	E	10	2	-	1/1/2/3	-
1	BRU	C	5	1	-	4/7/21/22	0/2/2/2
2	MVA	X	11	2	-	3/6/8/10	-
2	SAR	R	4	2	-	1/1/2/3	-
2	SAR	K	4	2	-	1/1/2/3	-
2	SAR	X	4	2	-	1/1/2/3	-
2	MVA	K	5	2	-	3/6/8/10	-
2	MVA	X	5	2	-	3/6/8/10	-
2	MVA	Q	11	2	-	2/6/8/10	-
1	BRU	G	5	1	-	0/7/21/22	0/2/2/2
2	SAR	F	4	2	-	1/1/2/3	-
2	MVA	E	11	2	-	3/6/8/10	-
1	BRU	P	5	1	-	0/7/21/22	0/2/2/2
1	BRU	D	5	1	-	2/7/21/22	0/2/2/2
1	BRU	O	5	1	-	4/7/21/22	0/2/2/2
2	MVA	W	5	2	-	3/6/8/10	-
2	SAR	Q	4	2	-	1/1/2/3	-
1	BRU	J	5	1	-	3/7/21/22	0/2/2/2
2	SAR	E	4	2	-	1/1/2/3	-
1	BRU	N	5	1	-	3/7/21/22	0/2/2/2
2	MVA	E	5	2	-	3/6/8/10	-
2	SAR	W	4	2	-	1/1/2/3	-
2	MVA	L	5	2	-	3/6/8/10	-
1	BRU	A	5	1	-	0/7/21/22	0/2/2/2
2	MVA	L	11	2	-	4/6/8/10	-
2	SAR	W	10	2	-	1/1/2/3	-
2	MVA	Q	5	2	-	3/6/8/10	-
1	BRU	I	5	1	-	4/7/21/22	0/2/2/2
1	BRU	T	5	1	-	1/7/21/22	0/2/2/2
2	SAR	X	10	2	-	1/1/2/3	-
2	MVA	R	5	2	-	5/6/8/10	-
2	SAR	F	10	2	-	1/1/2/3	-
2	SAR	Q	10	2	-	1/1/2/3	-
2	MVA	F	11	2	-	5/6/8/10	-
1	BRU	U	5	1	-	4/7/21/22	0/2/2/2
2	SAR	R	10	2	-	1/1/2/3	-
1	BRU	M	5	1	-	0/7/21/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAR	L	4	2	-	1/1/2/3	-
2	SAR	L	10	2	-	1/1/2/3	-
2	MVA	F	5	2	-	5/6/8/10	-
2	SAR	K	10	2	-	1/1/2/3	-
1	BRU	H	5	1	-	1/7/21/22	0/2/2/2

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	11	MVA	CB-CA-N	5.03	117.71	111.17
2	W	11	MVA	CB-CA-N	3.76	116.07	111.17
2	K	11	MVA	CB-CA-N	3.42	115.62	111.17
2	E	11	MVA	CB-CA-C	3.34	117.23	113.04
2	Q	11	MVA	CB-CA-N	3.12	115.23	111.17
1	C	5	BRU	BR-C5-C6	3.06	124.93	120.64
2	Q	5	MVA	CB-CA-C	2.93	116.71	113.04
1	B	5	BRU	C6-C5-C4	-2.67	117.96	120.67
1	N	5	BRU	C6-C5-C4	-2.66	117.97	120.67
1	M	5	BRU	C6-C5-C4	-2.62	118.01	120.67
1	O	5	BRU	C6-C5-C4	-2.59	118.05	120.67
1	P	5	BRU	C6-C5-C4	-2.52	118.11	120.67
2	W	11	MVA	CB-CA-C	2.51	116.19	113.04
2	X	11	MVA	CB-CA-N	2.51	114.44	111.17
1	J	5	BRU	C6-C5-C4	-2.50	118.14	120.67
1	D	5	BRU	C6-C5-C4	-2.45	118.19	120.67
1	N	5	BRU	BR-C5-C6	2.43	124.05	120.64
1	H	5	BRU	C6-C5-C4	-2.42	118.21	120.67
1	A	5	BRU	C6-C5-C4	-2.38	118.26	120.67
2	Q	10	SAR	O-C-CA	-2.37	118.56	125.42
2	Q	11	MVA	CB-CA-C	2.33	115.96	113.04
2	K	5	MVA	CB-CA-C	2.32	115.95	113.04
1	I	5	BRU	C6-C5-C4	-2.29	118.35	120.67
2	K	5	MVA	CB-CA-N	2.29	114.15	111.17
1	S	5	BRU	C6-C5-C4	-2.25	118.39	120.67
1	G	5	BRU	C6-C5-C4	-2.21	118.43	120.67
1	U	5	BRU	BR-C5-C6	2.21	123.74	120.64
1	T	5	BRU	C6-C5-C4	-2.17	118.47	120.67
1	V	5	BRU	C6-C5-C4	-2.16	118.48	120.67
2	R	4	SAR	O-C-CA	-2.12	119.27	125.42
2	W	5	MVA	CB-CA-C	2.11	115.69	113.04
2	E	5	MVA	CB-CA-C	2.11	115.69	113.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	5	BRU	C6-C5-C4	-2.10	118.54	120.67
2	K	10	SAR	O-C-CA	-2.08	119.40	125.42
2	W	4	SAR	O-C-CA	-2.05	119.50	125.42
2	X	4	SAR	O-C-CA	-2.04	119.53	125.42
1	T	5	BRU	O4-C4-C5	-2.03	123.29	125.84
1	C	5	BRU	C6-C5-C4	-2.03	118.61	120.67

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	SAR	C-CA-N-CN
2	E	5	MVA	N-CA-CB-CG2
2	E	10	SAR	C-CA-N-CN
2	E	11	MVA	C-CA-CB-CG1
2	F	5	MVA	N-CA-CB-CG1
2	F	5	MVA	N-CA-CB-CG2
2	F	5	MVA	C-CA-CB-CG2
2	F	10	SAR	C-CA-N-CN
2	F	11	MVA	N-CA-CB-CG1
2	F	11	MVA	N-CA-CB-CG2
2	F	11	MVA	C-CA-CB-CG2
2	K	4	SAR	C-CA-N-CN
2	K	5	MVA	N-CA-CB-CG2
2	K	10	SAR	C-CA-N-CN
2	L	5	MVA	CB-CA-N-CN
2	L	5	MVA	N-CA-CB-CG1
2	L	5	MVA	N-CA-CB-CG2
2	L	10	SAR	C-CA-N-CN
2	L	11	MVA	N-CA-CB-CG1
2	L	11	MVA	N-CA-CB-CG2
2	L	11	MVA	C-CA-CB-CG2
2	Q	4	SAR	C-CA-N-CN
2	Q	5	MVA	N-CA-CB-CG1
2	Q	5	MVA	N-CA-CB-CG2
2	Q	10	SAR	C-CA-N-CN
2	Q	11	MVA	C-CA-CB-CG1
2	R	5	MVA	CB-CA-N-CN
2	R	5	MVA	N-CA-CB-CG1
2	R	5	MVA	N-CA-CB-CG2
2	R	5	MVA	C-CA-CB-CG2
2	R	10	SAR	C-CA-N-CN

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Mol	Chain	Res	Type	Atoms
2	R	11	MVA	N-CA-CB-CG1
2	R	11	MVA	N-CA-CB-CG2
2	W	4	SAR	C-CA-N-CN
2	W	5	MVA	N-CA-CB-CG1
2	W	5	MVA	N-CA-CB-CG2
2	W	10	SAR	C-CA-N-CN
2	X	5	MVA	CB-CA-N-CN
2	X	5	MVA	N-CA-CB-CG1
2	X	10	SAR	C-CA-N-CN
2	X	11	MVA	N-CA-CB-CG1
2	X	11	MVA	N-CA-CB-CG2
1	I	5	BRU	C2'-C1'-N1-C2
1	U	5	BRU	O4'-C1'-N1-C6
1	C	5	BRU	C2'-C1'-N1-C2
1	O	5	BRU	C2'-C1'-N1-C2
1	O	5	BRU	O4'-C1'-N1-C6
1	U	5	BRU	C2'-C1'-N1-C2
1	C	5	BRU	O4'-C1'-N1-C6
1	I	5	BRU	C2'-C1'-N1-C6
1	I	5	BRU	O4'-C1'-N1-C6
1	U	5	BRU	O4'-C1'-N1-C2
1	O	5	BRU	O4'-C1'-N1-C2
1	C	5	BRU	C2'-C1'-N1-C6
1	O	5	BRU	C2'-C1'-N1-C6
2	E	11	MVA	C-CA-CB-CG2
2	F	5	MVA	C-CA-CB-CG1
2	R	5	MVA	C-CA-CB-CG1
1	C	5	BRU	O4'-C1'-N1-C2
2	E	5	MVA	N-CA-CB-CG1
2	K	5	MVA	N-CA-CB-CG1
1	H	5	BRU	C4'-C5'-O5'-P
1	N	5	BRU	C3'-C4'-C5'-O5'
1	I	5	BRU	O4'-C1'-N1-C2
1	U	5	BRU	C2'-C1'-N1-C6
1	B	5	BRU	C4'-C5'-O5'-P
1	N	5	BRU	C4'-C5'-O5'-P
1	T	5	BRU	C3'-C4'-C5'-O5'
2	E	5	MVA	CB-CA-N-CN
2	E	11	MVA	CB-CA-N-CN
2	F	5	MVA	CB-CA-N-CN
2	F	11	MVA	CB-CA-N-CN
2	K	5	MVA	CB-CA-N-CN

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Mol	Chain	Res	Type	Atoms
2	K	11	MVA	CB-CA-N-CN
2	L	11	MVA	CB-CA-N-CN
2	Q	5	MVA	CB-CA-N-CN
2	Q	11	MVA	CB-CA-N-CN
2	R	11	MVA	CB-CA-N-CN
2	W	5	MVA	CB-CA-N-CN
2	W	11	MVA	CB-CA-N-CN
2	X	11	MVA	CB-CA-N-CN
1	J	5	BRU	O4'-C1'-N1-C6
1	V	5	BRU	O4'-C1'-N1-C6
1	B	5	BRU	C3'-C4'-C5'-O5'
1	N	5	BRU	O4'-C4'-C5'-O5'
1	J	5	BRU	C2'-C1'-N1-C6
2	F	11	MVA	O-C-CA-CB
1	J	5	BRU	O4'-C1'-N1-C2
1	V	5	BRU	O4'-C1'-N1-C2
1	V	5	BRU	C2'-C1'-N1-C6
2	F	4	SAR	C-CA-N-CN
2	K	11	MVA	C-CA-CB-CG1
2	L	4	SAR	C-CA-N-CN
2	R	4	SAR	C-CA-N-CN
2	X	4	SAR	C-CA-N-CN
1	D	5	BRU	O4'-C1'-N1-C6
2	X	5	MVA	N-CA-CB-CG2
1	D	5	BRU	C2'-C1'-N1-C6

There are no ring outliers.

30 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	11	MVA	1	0
2	W	11	MVA	2	0
2	K	11	MVA	2	0
1	C	5	BRU	1	0
2	X	11	MVA	2	0
2	R	4	SAR	1	0
2	K	4	SAR	2	0
2	X	4	SAR	2	0
2	K	5	MVA	3	0
2	Q	11	MVA	3	0
2	F	4	SAR	1	0
2	E	11	MVA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	5	MVA	2	0
2	Q	4	SAR	2	0
2	E	4	SAR	2	0
2	E	5	MVA	3	0
2	W	4	SAR	2	0
2	L	11	MVA	2	0
2	Q	5	MVA	3	0
1	I	5	BRU	1	0
1	T	5	BRU	2	0
2	X	10	SAR	2	0
2	R	5	MVA	1	0
2	F	10	SAR	2	0
2	F	11	MVA	1	0
2	R	10	SAR	2	0
2	L	4	SAR	2	0
2	L	10	SAR	2	0
2	F	5	MVA	1	0
2	K	10	SAR	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.