



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:42 AM GMT

PDB ID : 3MQ6
Title : Domain swapped SgrAI with DNA and calcium bound
Authors : Dunten, P.W.; Horton, N.C.; Little, E.J.
Deposited on : 2010-04-27
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

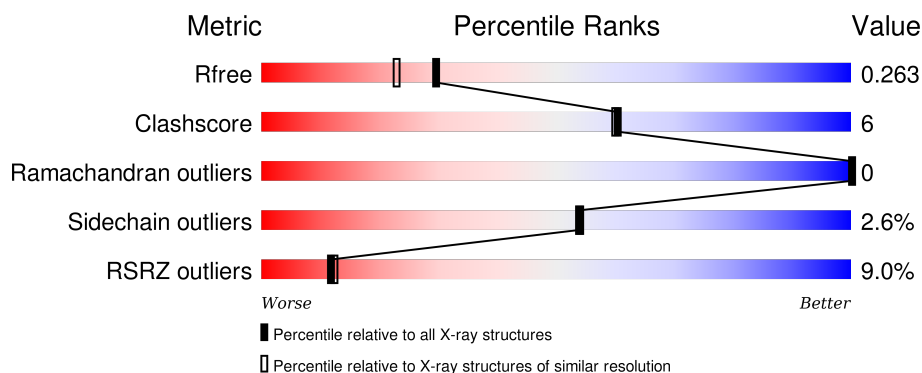
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	338	<div> <div>8%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	B	338	<div> <div>9%</div> <div>83%</div> <div>17%</div> <div>.</div> </div>
1	C	338	<div> <div>7%</div> <div>87%</div> <div>12%</div> <div>..</div> </div>
1	D	338	<div> <div>7%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	E	338	<div> <div>8%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	338	
1	G	338	
1	H	338	
2	K	17	
2	L	17	
2	M	17	
2	N	17	
2	O	17	
2	P	17	
2	Q	17	
2	R	17	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25250 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 SgrIR restriction enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2612	1653	461	489	9			
1	B	338	Total	C	N	O	S	0	0	0
			2658	1681	473	495	9			
1	C	335	Total	C	N	O	S	0	2	0
			2654	1679	476	490	9			
1	D	333	Total	C	N	O	S	0	1	0
			2628	1665	465	489	9			
1	E	333	Total	C	N	O	S	0	1	0
			2645	1673	470	493	9			
1	F	338	Total	C	N	O	S	0	0	0
			2652	1678	470	495	9			
1	G	335	Total	C	N	O	S	0	0	0
			2644	1674	470	491	9			
1	H	336	Total	C	N	O	S	0	1	1
			2653	1681	472	491	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	ASP	ASN	CLONING ARTIFACT	UNP Q9F6L0
B	63	ASP	ASN	CLONING ARTIFACT	UNP Q9F6L0
C	63	ASP	ASN	CLONING ARTIFACT	UNP Q9F6L0
D	63	ASP	ASN	CLONING ARTIFACT	UNP Q9F6L0
E	63	ASP	ASN	CLONING ARTIFACT	UNP Q9F6L0
F	63	ASP	ASN	CLONING ARTIFACT	UNP Q9F6L0
G	63	ASP	ASN	CLONING ARTIFACT	UNP Q9F6L0
H	63	ASP	ASN	CLONING ARTIFACT	UNP Q9F6L0

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	17	Total 346	C 165	N 66	O 99	P 16	0	0	0
2	K	17	Total 346	C 165	N 66	O 99	P 16	0	0	0
2	N	17	Total 346	C 165	N 66	O 99	P 16	0	0	0
2	M	17	Total 346	C 165	N 66	O 99	P 16	0	0	0
2	P	16	Total 325	C 155	N 61	O 94	P 15	0	0	0
2	O	17	Total 346	C 165	N 66	O 99	P 16	0	0	0
2	R	17	Total 346	C 165	N 66	O 99	P 16	0	0	0
2	Q	17	Total 346	C 165	N 66	O 99	P 16	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total 2	Ca 2	0	0
3	D	3	Total 3	Ca 3	0	0
3	E	2	Total 2	Ca 2	0	0
3	H	3	Total 3	Ca 3	0	0
3	B	3	Total 3	Ca 3	0	0
3	C	3	Total 3	Ca 3	0	0
3	A	3	Total 3	Ca 3	0	0
3	F	3	Total 3	Ca 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total 135	O 135	0	0
4	B	133	Total 133	O 133	0	0

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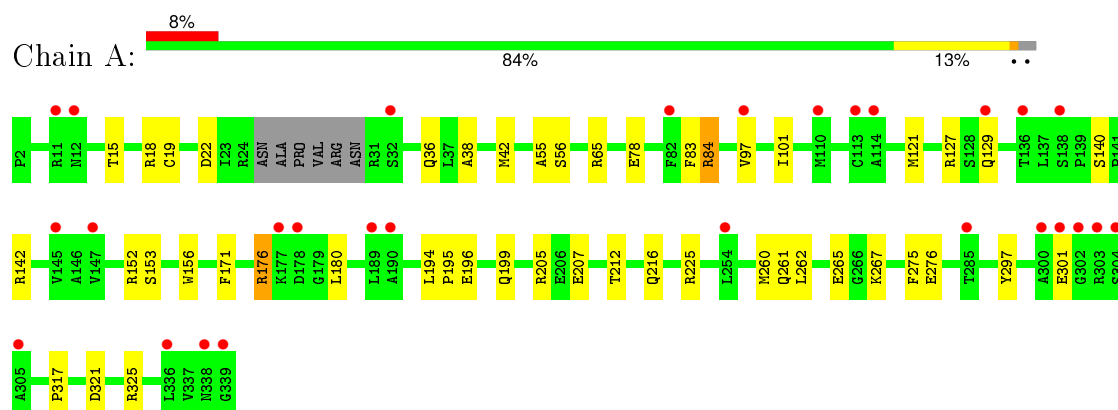
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	132	Total 132	O 132	0	0
4	D	161	Total 161	O 161	0	0
4	E	169	Total 169	O 169	0	0
4	F	151	Total 151	O 151	0	0
4	G	140	Total 140	O 140	0	0
4	H	135	Total 135	O 135	0	0
4	L	25	Total 25	O 25	0	0
4	K	24	Total 24	O 24	0	0
4	N	22	Total 22	O 22	0	0
4	M	19	Total 19	O 19	0	0
4	P	26	Total 26	O 26	0	0
4	O	22	Total 22	O 22	0	0
4	R	20	Total 20	O 20	0	0
4	Q	21	Total 21	O 21	0	0

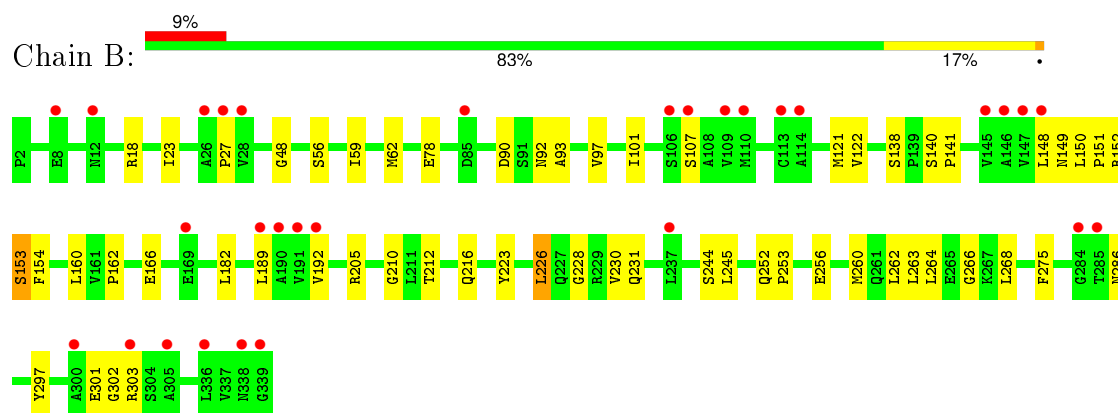
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

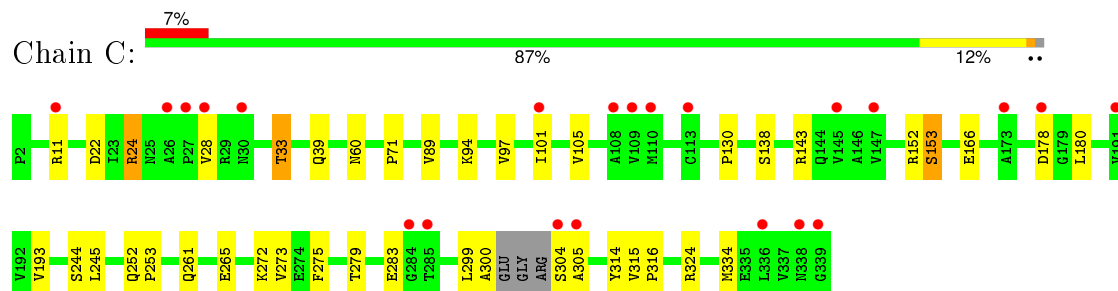
- Molecule 1: SgrAIR restriction enzyme



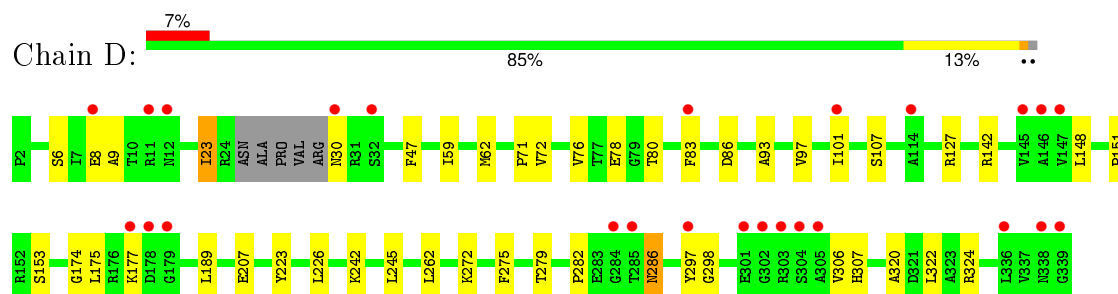
- Molecule 1: SgrAIR restriction enzyme



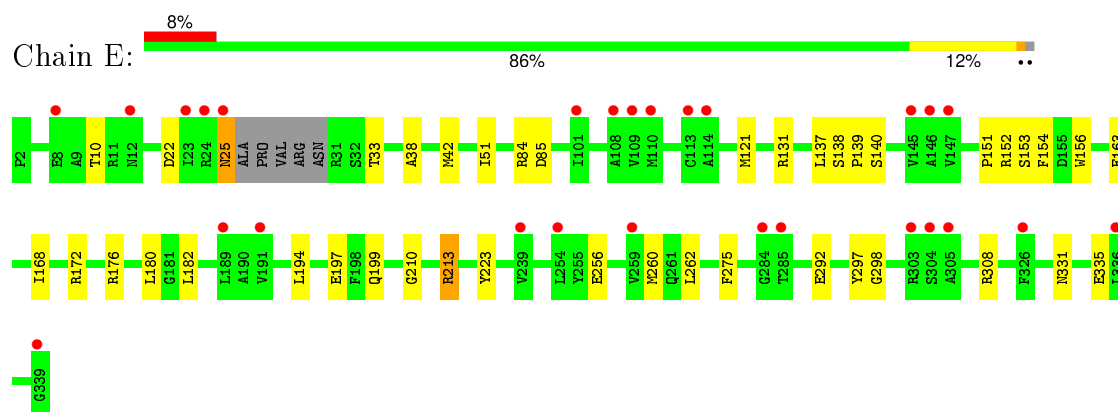
- Molecule 1: SgrAIR restriction enzyme



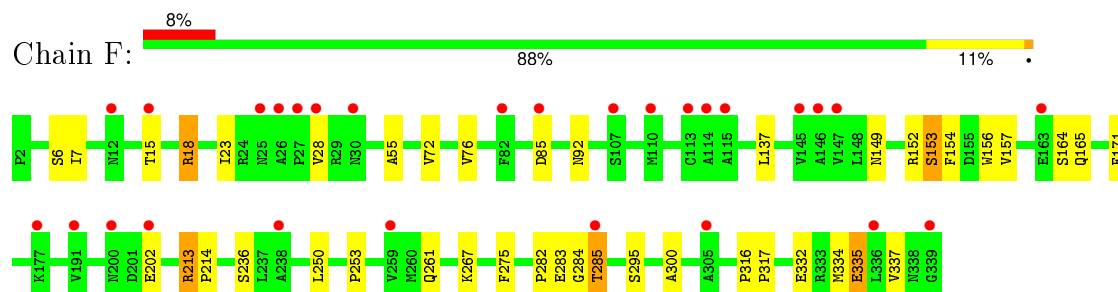
- Molecule 1: SgrAIR restriction enzyme



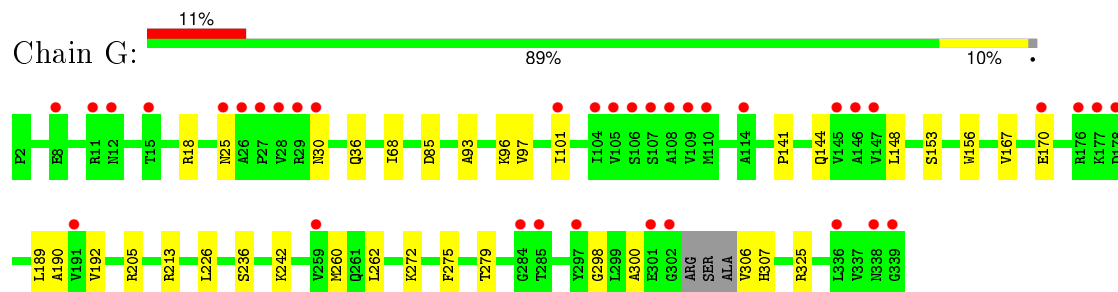
- Molecule 1: SgrAIR restriction enzyme



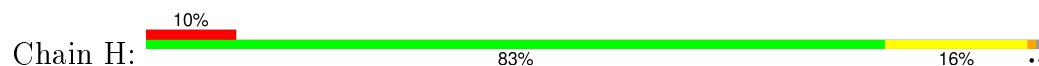
- Molecule 1: SgrAIR restriction enzyme

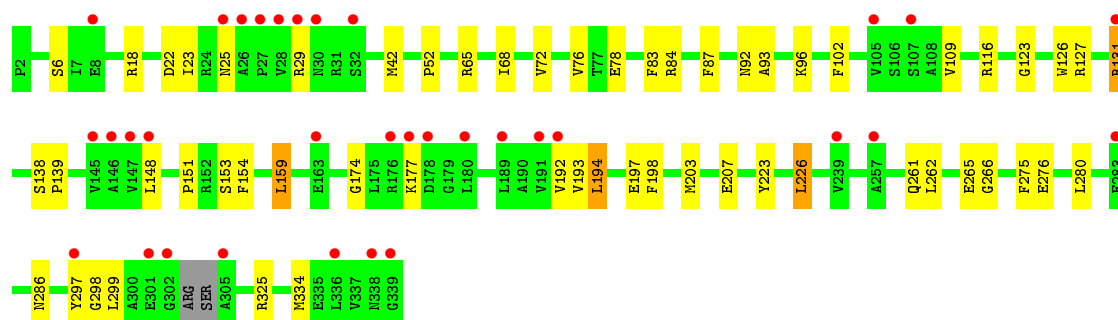


- Molecule 1: SgrAIR restriction enzyme

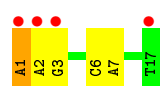


- Molecule 1: SgrAIR restriction enzyme





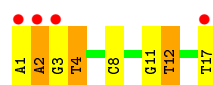
- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')



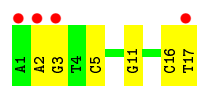
- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')



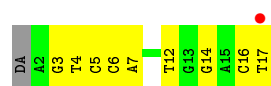
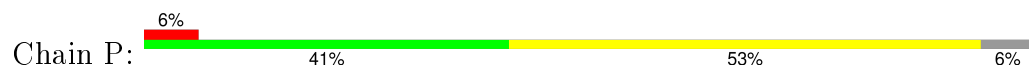
- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')



- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*
*T)-3')

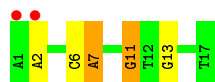


- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')



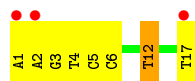
- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')

Chain O: 



- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')

Chain R: 



- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')

Chain Q: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.38Å 134.95Å 237.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.46 – 2.00 25.46 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.8 (25.46-2.00) 94.9 (25.46-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.211 , 0.261 0.208 , 0.263	Depositor DCC
R_{free} test set	5402 reflections (2.03%)	DCC
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.7	EDS
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	25 of 266875 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25250	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA

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	0.38	0/2669	0.56	0/3623
1	B	0.38	0/2717	0.52	0/3690
1	C	0.41	0/2713	0.57	0/3684
1	D	0.42	0/2686	0.56	0/3646
1	E	0.43	0/2703	0.57	0/3667
1	F	0.41	0/2711	0.58	0/3683
1	G	0.38	0/2702	0.55	0/3667
1	H	0.39	0/2712	0.58	0/3683
2	K	0.83	0/388	1.56	9/597 (1.5%)
2	L	0.83	0/388	1.45	4/597 (0.7%)
2	M	0.81	0/388	1.38	2/597 (0.3%)
2	N	0.78	0/388	1.43	5/597 (0.8%)
2	O	0.84	0/388	1.63	5/597 (0.8%)
2	P	0.88	0/364	1.63	5/560 (0.9%)
2	Q	0.77	0/388	1.46	4/597 (0.7%)
2	R	0.79	0/388	1.55	8/597 (1.3%)
All	All	0.47	0/24693	0.77	42/34082 (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	F	0	1

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	6	DC	O4'-C1'-N1	-13.19	98.77	108.00
2	P	5	DC	O4'-C1'-N1	-10.03	100.98	108.00
2	R	12	DT	O4'-C4'-C3'	-9.36	100.39	106.00
2	O	6	DC	O4'-C1'-N1	-8.77	101.86	108.00
2	N	11	DG	O4'-C1'-N9	-8.59	101.99	108.00
2	R	6	DC	O4'-C1'-N1	-7.88	102.48	108.00
2	M	5	DC	O4'-C1'-N1	-7.53	102.73	108.00
2	K	11	DG	O4'-C1'-N9	-7.35	102.86	108.00
2	Q	6	DC	O4'-C1'-N1	-7.29	102.89	108.00
2	R	12	DT	C1'-O4'-C4'	-7.15	102.95	110.10
2	N	12	DT	C1'-O4'-C4'	-7.12	102.98	110.10
2	L	1	DA	P-O3'-C3'	6.60	127.62	119.70
2	L	6	DC	O4'-C1'-N1	-6.45	103.48	108.00
2	K	12	DT	C1'-O4'-C4'	-6.17	103.93	110.10
2	O	13	DG	O4'-C1'-N9	-6.17	103.68	108.00
2	K	16	DC	O4'-C1'-N1	6.05	112.24	108.00
2	N	2	DA	P-O3'-C3'	6.05	126.96	119.70
2	P	14	DG	O4'-C1'-N9	-6.00	103.80	108.00
2	L	7	DA	P-O3'-C3'	5.90	126.78	119.70
2	O	7	DA	P-O3'-C3'	5.90	126.78	119.70
2	M	11	DG	P-O3'-C3'	5.86	126.73	119.70
2	R	12	DT	N3-C2-O2	5.83	125.80	122.30
2	O	2	DA	C3'-C2'-C1'	-5.75	95.60	102.50
2	R	5	DC	O4'-C1'-N1	-5.68	104.03	108.00
2	Q	11	DG	O4'-C1'-N9	-5.61	104.07	108.00
2	N	8	DC	O4'-C4'-C3'	-5.56	102.28	104.50
2	L	6	DC	P-O3'-C3'	5.52	126.33	119.70
2	K	7	DA	P-O3'-C3'	5.48	126.28	119.70
2	P	6	DC	P-O3'-C3'	5.48	126.28	119.70
2	K	4	DT	N3-C4-O4	5.44	123.17	119.90
2	N	4	DT	N3-C4-O4	5.38	123.13	119.90
2	Q	16	DC	C1'-O4'-C4'	-5.30	104.80	110.10
2	P	12	DT	O4'-C1'-N1	-5.24	104.33	108.00
2	K	1	DA	C4'-C3'-C2'	-5.17	98.44	103.10
2	K	4	DT	C5-C4-O4	-5.15	121.30	124.90
2	O	11	DG	O4'-C1'-N9	-5.09	104.44	108.00
2	K	1	DA	C3'-C2'-C1'	-5.08	96.40	102.50
2	R	4	DT	C5-C4-O4	-5.08	121.34	124.90
2	P	7	DA	P-O3'-C3'	5.05	125.76	119.70
2	Q	7	DA	P-O3'-C3'	5.04	125.75	119.70
2	R	12	DT	C5-C4-O4	-5.01	121.39	124.90
2	R	4	DT	N3-C4-O4	5.01	122.91	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	284	GLY	Peptide

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	2612	0	2560	30	0
1	B	2658	0	2614	35	0
1	C	2654	0	2607	27	0
1	D	2628	0	2577	40	0
1	E	2645	0	2598	34	0
1	F	2652	0	2603	26	0
1	G	2644	0	2605	23	0
1	H	2653	0	2608	39	0
2	K	346	0	192	6	0
2	L	346	0	192	6	0
2	M	346	0	192	6	0
2	N	346	0	192	8	0
2	O	346	0	192	2	0
2	P	325	0	181	3	0
2	Q	346	0	192	6	0
2	R	346	0	192	7	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
3	F	3	0	0	0	0
3	G	2	0	0	0	0
3	H	3	0	0	0	0
4	A	135	0	0	6	0
4	B	133	0	0	0	0
4	C	132	0	0	1	0
4	D	161	0	0	4	0
4	E	169	0	0	2	0
4	F	151	0	0	3	0
4	G	140	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	135	0	0	1	0
4	K	24	0	0	0	0
4	L	25	0	0	0	0
4	M	19	0	0	0	0
4	N	22	0	0	0	0
4	O	22	0	0	0	0
4	P	26	0	0	0	0
4	Q	21	0	0	0	0
4	R	20	0	0	0	0
All	All	25250	0	22297	259	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 6.

All (259) 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:D:174:GLY:O	1:D:177:LYS:HG2	1.83	0.77
1:H:148:LEU:HD21	1:H:226:LEU:HD13	1.66	0.76
1:E:297[B]:TYR:CG	1:E:298:GLY:N	2.57	0.73
1:B:301:GLU:HG3	1:B:302:GLY:H	1.53	0.72
1:D:76:VAL:O	1:D:80:THR:HG23	1.95	0.67
1:G:167:VAL:O	1:G:170:GLU:HG3	1.94	0.67
1:G:298:GLY:O	1:G:306:VAL:HG22	1.94	0.67
2:M:2:DA:H2''	2:M:3:DG:OP2	1.96	0.66
1:D:93:ALA:HA	2:N:12:DT:H4'	1.78	0.66
1:C:300:ALA:HB2	1:D:297[A]:TYR:CE1	2.30	0.65
1:F:285:THR:O	1:F:285:THR:HG23	1.97	0.65
1:H:154:PHE:HZ	1:H:159:LEU:HD13	1.62	0.64
1:G:189:LEU:HD23	1:G:190:ALA:N	2.12	0.63
1:B:301:GLU:HG3	1:B:302:GLY:N	2.14	0.63
1:E:121:MET:HB3	1:E:140:SER:O	2.01	0.60
1:E:262:LEU:HD23	1:E:262:LEU:C	2.22	0.60
2:R:17:DT:H3	2:Q:2:DA:H61	1.49	0.59
1:C:252:GLN:HB3	1:C:253:PRO:HD3	1.85	0.59
1:E:297[B]:TYR:CD2	1:E:298:GLY:N	2.71	0.58
1:E:137:LEU:HD13	1:E:335:GLU:HG2	1.86	0.58
1:B:266:GLY:HA2	1:B:297:TYR:OH	2.03	0.58
1:B:23:ILE:HD13	1:G:36:GLN:HG3	1.85	0.58
1:B:122:VAL:HG21	1:B:205:ARG:HD3	1.86	0.58
2:L:2:DA:H61	2:K:17:DT:H3	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:GLU:O	1:F:335:GLU:HB2	2.03	0.57
1:D:97:VAL:HG12	1:D:101:ILE:HD12	1.86	0.57
1:E:151:PRO:HG3	1:E:223:TYR:CZ	2.39	0.57
1:H:52:PRO:O	1:H:109:VAL:HG22	2.04	0.57
1:B:48:GLY:O	1:B:210:GLY:HA3	2.05	0.56
1:G:272:LYS:HG3	1:G:307:HIS:CD2	2.40	0.56
1:D:272:LYS:HG3	1:D:307:HIS:CD2	2.40	0.56
1:G:189:LEU:C	1:G:189:LEU:HD23	2.26	0.56
2:R:17:DT:H3	2:Q:2:DA:N6	2.03	0.56
1:E:137:LEU:CD1	1:E:335:GLU:HG2	2.36	0.55
1:F:282:PRO:HD2	1:F:283:GLU:OE2	2.07	0.55
1:D:59:ILE:HA	1:D:62:MET:HE3	1.88	0.55
1:F:261:GLN:OE1	1:F:295:SER:HB2	2.07	0.55
2:Q:2:DA:H1'	2:Q:3:DG:C8	2.41	0.55
1:E:151:PRO:HD2	1:E:154:PHE:HB2	1.89	0.55
1:D:286:ASN:HB2	4:D:874:HOH:O	2.05	0.55
1:D:93:ALA:HB2	2:N:12:DT:H5''	1.90	0.54
2:K:1:DA:H2''	2:K:2:DA:N7	2.23	0.54
1:G:93:ALA:HA	2:R:12:DT:H4'	1.90	0.54
1:H:154:PHE:CZ	1:H:159:LEU:HD13	2.41	0.53
1:A:317:PRO:HD2	1:A:321:ASP:HB3	1.90	0.53
2:N:17:DT:O2	2:M:2:DA:N1	2.41	0.53
1:A:129:GLN:HG3	1:A:129:GLN:O	2.08	0.53
1:B:182:LEU:HD23	1:B:263:LEU:HD21	1.90	0.53
2:N:17:DT:H3	2:M:2:DA:H61	1.55	0.53
1:D:245:LEU:HD12	1:D:282:PRO:HA	1.91	0.53
2:R:2:DA:H2''	2:R:3:DG:OP2	2.08	0.53
1:G:148:LEU:HD21	1:G:226:LEU:HD13	1.90	0.53
1:B:97:VAL:HG12	1:B:101:ILE:HD12	1.91	0.53
1:A:261:GLN:HG2	1:A:265:GLU:OE2	2.08	0.53
1:F:7:ILE:HG22	4:F:1222:HOH:O	2.09	0.52
1:C:324[B]:ARG:HH11	1:C:324[B]:ARG:HG2	1.73	0.52
1:A:83:PHE:C	1:A:84:ARG:HG2	2.30	0.52
1:E:297[A]:TYR:CD1	1:F:300:ALA:HB2	2.45	0.52
1:D:23:ILE:HG23	1:D:23:ILE:O	2.08	0.52
1:B:148:LEU:HD21	1:B:226:LEU:HD13	1.92	0.52
1:E:131:ARG:HG3	4:E:369:HOH:O	2.10	0.52
1:A:65:ARG:HG3	4:A:441:HOH:O	2.10	0.52
1:D:83:PHE:CZ	1:E:22:ASP:HB2	2.45	0.52
1:F:15:THR:HA	1:F:18:ARG:HG3	1.92	0.51
1:B:262:LEU:HD23	1:B:262:LEU:C	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:SER:OG	1:B:59:ILE:HG13	2.11	0.51
1:F:334:MET:HE1	1:F:337:VAL:HG21	1.93	0.51
1:D:148:LEU:HD21	1:D:226:LEU:HD22	1.93	0.51
1:E:163:GLU:H	1:E:163:GLU:CD	2.13	0.51
1:D:322:LEU:HD12	4:D:907:HOH:O	2.11	0.51
1:C:71:PRO:HB2	1:C:101:ILE:HD13	1.93	0.51
2:L:2:DA:N1	2:K:17:DT:O2	2.43	0.51
1:H:151:PRO:HG3	1:H:223:TYR:CZ	2.46	0.50
2:L:1:DA:N3	2:L:1:DA:H2'	2.26	0.50
1:G:192:VAL:HG21	1:G:226:LEU:HD22	1.92	0.50
1:B:264:LEU:HD23	1:B:268:LEU:HD12	1.93	0.50
1:F:157:VAL:HG12	1:F:165:GLN:HG2	1.93	0.50
1:B:256:GLU:O	1:B:260:MET:HG3	2.11	0.50
1:A:78:GLU:OE2	1:H:18:ARG:HB3	2.11	0.50
1:H:192:VAL:HG21	1:H:226:LEU:HD22	1.93	0.50
1:A:38:ALA:O	1:A:42:MET:HG3	2.12	0.49
1:H:193:VAL:HG22	1:H:334:MET:HE1	1.94	0.49
1:B:212:THR:O	1:B:216:GLN:HG3	2.12	0.49
1:H:93:ALA:HB2	2:Q:12:DT:H4'	1.94	0.49
1:E:151:PRO:HG3	1:E:223:TYR:CE1	2.48	0.49
1:E:194:LEU:HD23	1:E:199:GLN:HA	1.95	0.49
1:A:83:PHE:CZ	1:H:22:ASP:HB2	2.47	0.49
1:G:97:VAL:O	1:G:101:ILE:HG12	2.12	0.49
1:E:176:ARG:HA	1:E:180:LEU:O	2.13	0.49
1:C:39:GLN:HB3	1:C:97:VAL:HG13	1.94	0.49
1:A:127:ARG:NH1	1:A:207:GLU:HG3	2.28	0.49
1:B:160:LEU:O	1:B:228:GLY:HA2	2.12	0.49
1:C:283:GLU:HA	1:C:283:GLU:OE1	2.13	0.49
1:E:154:PHE:CE2	1:E:156:TRP:HA	2.48	0.49
1:D:151:PRO:HG3	1:D:223:TYR:CZ	2.48	0.48
2:N:2:DA:H2''	2:N:3:DG:OP2	2.13	0.48
1:D:297[B]:TYR:HB3	4:D:381:HOH:O	2.14	0.48
1:B:121:MET:HB3	1:B:140:SER:O	2.13	0.48
1:A:176:ARG:HA	1:A:180:LEU:O	2.13	0.48
1:F:171:PHE:CE1	1:F:267:LYS:HE3	2.48	0.48
1:D:72:VAL:HG23	4:D:354:HOH:O	2.13	0.48
1:H:262:LEU:HD23	1:H:262:LEU:C	2.35	0.47
1:F:250:LEU:O	1:F:253:PRO:HD2	2.14	0.47
1:C:314:TYR:CE2	1:C:316:PRO:HB3	2.49	0.47
2:R:1:DA:H3'	2:R:2:DA:C8	2.49	0.47
1:F:92:ASN:HB3	2:O:11:DG:N3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:GLN:HG2	1:C:273:VAL:HB	1.96	0.47
1:A:97:VAL:HG12	1:A:101:ILE:HD12	1.95	0.47
1:E:84:ARG:HB3	1:E:85:ASP:H	1.59	0.47
1:A:18:ARG:HB3	1:H:78:GLU:OE2	2.15	0.47
1:B:244:SER:C	1:B:245:LEU:HD23	2.35	0.47
1:G:325:ARG:HH11	1:G:325:ARG:HG2	1.80	0.47
1:A:18:ARG:HD3	4:A:372:HOH:O	2.15	0.47
1:B:152:ARG:O	1:B:153:SER:CB	2.62	0.47
1:H:116:ARG:HG2	1:H:126:TRP:CZ3	2.50	0.47
1:F:154:PHE:CE2	1:F:156:TRP:HA	2.49	0.47
1:H:194:LEU:HD22	1:H:198:PHE:HB2	1.96	0.47
2:M:17:DT:H3'	2:M:17:DT:H6	1.79	0.46
1:C:60:ASN:HD21	1:C:130:PRO:HG3	1.80	0.46
1:E:38:ALA:O	1:E:42:MET:HG3	2.15	0.46
1:E:138:SER:HA	1:E:139:PRO:HD3	1.79	0.46
1:H:138:SER:HA	1:H:139:PRO:HD3	1.78	0.46
1:B:151:PRO:HG2	1:B:154:PHE:HB2	1.97	0.46
1:H:92:ASN:HB3	2:Q:11:DG:N3	2.31	0.46
2:K:2:DA:H2''	2:K:3:DG:OP2	2.16	0.46
1:F:72:VAL:O	1:F:76:VAL:HG23	2.15	0.46
1:E:262:LEU:O	1:E:262:LEU:HD23	2.16	0.46
1:D:97:VAL:CG1	1:D:101:ILE:HD12	2.46	0.46
1:C:28:VAL:HG13	1:C:28:VAL:O	2.16	0.46
1:A:205:ARG:NH1	4:A:1235:HOH:O	2.48	0.45
2:P:3:DG:H2'	2:P:4:DT:H72	1.97	0.45
2:L:2:DA:H1'	2:L:3:DG:C5'	2.46	0.45
1:C:180:LEU:CD1	1:D:306:VAL:HG12	2.46	0.45
2:L:2:DA:H2''	2:L:3:DG:OP2	2.16	0.45
1:D:127:ARG:HD2	1:D:207:GLU:OE2	2.16	0.45
1:D:320:ALA:O	1:D:324:ARG:HG3	2.16	0.45
1:B:90:ASP:OD2	1:B:92:ASN:HB2	2.17	0.45
1:A:194:LEU:HD12	1:A:195:PRO:HD2	1.98	0.45
1:G:141:PRO:O	1:G:144:GLN:HG3	2.17	0.45
1:C:138:SER:O	1:C:143:ARG:NH1	2.48	0.45
1:H:83:PHE:HB2	1:H:87:PHE:HB2	1.98	0.45
1:C:60:ASN:ND2	1:C:130:PRO:HG3	2.32	0.45
1:C:152:ARG:O	1:C:153:SER:CB	2.64	0.45
1:H:65:ARG:HA	1:H:280:LEU:HD13	1.99	0.45
1:D:297[B]:TYR:CD2	1:D:298:GLY:N	2.85	0.45
1:D:72:VAL:O	1:D:76:VAL:HG23	2.17	0.45
1:H:151:PRO:HG2	1:H:154:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:HB2	4:A:892:HOH:O	2.17	0.44
1:H:131:ARG:H	1:H:131:ARG:HG2	1.58	0.44
1:B:303:ARG:HA	1:B:303:ARG:HD3	1.74	0.44
1:B:244:SER:O	1:B:245:LEU:HD23	2.17	0.44
1:A:55:ALA:HB1	4:A:1285:HOH:O	2.16	0.44
1:D:107:SER:OG	1:D:189:LEU:HD12	2.17	0.44
1:D:6:SER:HB3	1:D:9:ALA:HB3	1.99	0.44
1:H:96:LYS:HG3	2:Q:12:DT:O2	2.18	0.44
2:P:16:DC:H2''	2:P:17:DT:OP2	2.17	0.44
1:E:168:ILE:HG22	1:E:172:ARG:HD2	2.00	0.44
1:D:262:LEU:C	1:D:262:LEU:HD23	2.38	0.44
1:B:78:GLU:OE2	1:G:18:ARG:HB3	2.18	0.44
1:D:226:LEU:N	1:D:226:LEU:HD12	2.33	0.44
1:H:194:LEU:HD23	1:H:194:LEU:HA	1.84	0.44
1:A:22:ASP:HB2	1:H:83:PHE:CZ	2.52	0.44
1:D:83:PHE:O	1:D:86:ASP:HB2	2.18	0.43
1:C:324[B]:ARG:NH1	1:C:324[B]:ARG:HG2	2.33	0.43
1:D:23:ILE:HG22	1:E:33:THR:O	2.18	0.43
1:A:36:GLN:HB2	1:H:23:ILE:HD13	2.00	0.43
1:B:162:PRO:O	1:B:166:GLU:HG3	2.19	0.43
1:F:152:ARG:O	1:F:153:SER:CB	2.66	0.43
1:C:89:VAL:HG23	1:C:94:LYS:HE3	2.00	0.43
2:M:2:DA:C2'	2:M:3:DG:OP2	2.65	0.43
1:D:242:LYS:O	1:D:279:THR:HA	2.19	0.43
2:M:16:DC:H2''	2:M:17:DT:H5'	2.00	0.43
1:B:93:ALA:HA	2:K:12:DT:H4'	2.01	0.43
2:N:1:DA:H4'	2:N:2:DA:O5'	2.19	0.43
1:H:83:PHE:C	1:H:84:ARG:HG2	2.38	0.43
1:E:292:GLU:HG2	1:E:308:ARG:NH2	2.34	0.43
1:H:148:LEU:CD2	1:H:226:LEU:HD13	2.41	0.43
2:K:12:DT:H2'	2:K:13:DG:N7	2.34	0.43
1:B:149:ASN:C	1:B:149:ASN:OD1	2.58	0.43
2:L:2:DA:H1'	2:L:3:DG:H5'	2.01	0.42
1:H:262:LEU:O	1:H:266:GLY:HA3	2.19	0.42
1:A:171:PHE:CE1	1:A:267:LYS:HE3	2.54	0.42
1:F:55:ALA:HB1	4:F:1317:HOH:O	2.18	0.42
1:E:197:GLU:H	1:E:197:GLU:CD	2.21	0.42
1:H:174:GLY:O	1:H:177:LYS:HG2	2.18	0.42
1:C:299:LEU:HD21	1:D:175:LEU:HD21	2.01	0.42
1:E:297[A]:TYR:CE1	1:F:300:ALA:HA	2.55	0.42
1:F:285:THR:O	1:F:285:THR:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:LEU:HD13	1:F:335:GLU:HG2	2.01	0.42
1:G:93:ALA:HB2	2:R:12:DT:C5'	2.48	0.42
1:C:180:LEU:HD13	1:D:306:VAL:HG12	2.01	0.42
1:H:261:GLN:HG2	1:H:265:GLU:OE2	2.19	0.42
1:E:213:ARG:HD2	1:E:213:ARG:HA	1.68	0.42
1:A:152:ARG:O	1:A:153:SER:CB	2.68	0.42
1:E:331:ASN:HB3	4:E:348:HOH:O	2.19	0.42
1:G:68:ILE:HD13	1:G:68:ILE:HA	1.84	0.42
1:G:213:ARG:HD3	4:G:927:HOH:O	2.19	0.42
1:C:304:SER:OG	1:C:305:ALA:N	2.52	0.42
1:D:47:PHE:HE2	1:D:71:PRO:CG	2.33	0.42
1:G:242:LYS:O	1:G:279:THR:HA	2.20	0.42
1:B:27:PRO:HG2	1:G:25:ASN:HB2	2.02	0.42
1:G:262:LEU:HD23	1:G:262:LEU:C	2.40	0.42
1:H:276:GLU:CD	1:H:325:ARG:HH12	2.20	0.42
1:B:150:LEU:HD22	1:B:154:PHE:CE2	2.55	0.42
1:F:152:ARG:O	1:F:153:SER:HB2	2.20	0.42
1:C:244:SER:C	1:C:245:LEU:HD23	2.40	0.42
1:F:213:ARG:N	1:F:214:PRO:CD	2.83	0.42
1:C:193:VAL:HG22	1:C:334:MET:HE1	2.01	0.41
1:F:28:VAL:HG13	1:F:28:VAL:O	2.18	0.41
1:E:256:GLU:O	1:E:260:MET:HG3	2.19	0.41
1:H:127:ARG:HH21	1:H:207:GLU:HG3	1.84	0.41
1:C:101:ILE:O	1:C:105:VAL:HG23	2.20	0.41
1:F:6:SER:HB2	4:F:618:HOH:O	2.19	0.41
1:F:149:ASN:OD1	1:F:149:ASN:C	2.59	0.41
1:E:25:ASN:C	1:E:25:ASN:HD22	2.24	0.41
1:D:78:GLU:HG3	1:E:10:THR:HG21	2.01	0.41
1:D:297[B]:TYR:CG	1:D:298:GLY:N	2.86	0.41
1:A:212:THR:O	1:A:216:GLN:HG3	2.19	0.41
1:E:51:ILE:CD1	1:E:210:GLY:HA2	2.51	0.41
1:G:156:TRP:CE2	1:G:260:MET:HG2	2.55	0.41
1:D:71:PRO:HB2	1:D:101:ILE:HD13	2.02	0.41
1:B:151:PRO:HG3	1:B:223:TYR:CZ	2.55	0.41
1:B:192:VAL:HG21	1:B:226:LEU:HD22	2.01	0.41
1:H:72:VAL:O	1:H:76:VAL:HG23	2.20	0.41
1:A:19:CYS:HB3	1:H:42:MET:HG2	2.03	0.41
1:D:47:PHE:CE2	1:D:71:PRO:HG3	2.55	0.41
1:C:272:LYS:CE	4:C:379:HOH:O	2.67	0.41
1:G:96:LYS:HG3	2:R:12:DT:O2	2.20	0.41
1:C:261:GLN:O	1:C:265:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:HA	1:A:195:PRO:HD3	1.87	0.41
1:A:156:TRP:CE2	1:A:260:MET:HG2	2.55	0.41
1:D:93:ALA:CA	2:N:12:DT:H4'	2.46	0.41
1:B:107:SER:OG	1:B:189:LEU:HD12	2.20	0.41
1:C:22:ASP:OD2	1:C:24:ARG:HG2	2.21	0.41
1:C:33:THR:HB	1:F:23:ILE:HD11	2.02	0.41
1:A:262:LEU:C	1:A:262:LEU:HD23	2.40	0.41
1:D:23:ILE:CG2	1:D:23:ILE:O	2.68	0.41
1:B:140:SER:HA	1:B:141:PRO:HD3	1.89	0.41
1:G:300:ALA:HB2	1:H:297[A]:TYR:CD1	2.56	0.41
1:H:297[B]:TYR:CG	1:H:298:GLY:N	2.85	0.41
1:H:197:GLU:H	1:H:197:GLU:CD	2.22	0.41
1:B:230:VAL:HG12	1:B:231:GLN:O	2.21	0.41
1:H:68:ILE:HD12	1:H:102:PHE:HA	2.02	0.41
1:F:316:PRO:HA	1:F:317:PRO:HD3	1.87	0.41
2:N:3:DG:H2''	2:N:4:DT:OP2	2.20	0.41
1:A:225:ARG:HD3	4:A:1196:HOH:O	2.21	0.41
1:H:123:GLY:HA2	4:H:1280:HOH:O	2.21	0.41
1:D:23:ILE:CG2	1:E:33:THR:O	2.69	0.40
2:P:17:DT:H2'	2:P:17:DT:OP2	2.21	0.40
1:A:121:MET:HB3	1:A:140:SER:O	2.20	0.40
1:C:279:THR:O	1:C:315:VAL:HA	2.21	0.40
1:E:182:LEU:HD12	1:E:182:LEU:HA	1.84	0.40
1:G:325:ARG:HG2	1:G:325:ARG:NH1	2.36	0.40
1:A:196:GLU:HA	1:A:199:GLN:NE2	2.36	0.40
1:E:152:ARG:HG2	2:O:7:DA:H5'	2.03	0.40
1:B:252:GLN:N	1:B:253:PRO:CD	2.84	0.40
1:B:59:ILE:HA	1:B:62:MET:HE3	2.03	0.40
1:A:276:GLU:CD	1:A:325:ARG:HH12	2.24	0.40
1:H:299:LEU:HA	1:H:299:LEU:HD23	1.85	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	328/338 (97%)	316 (96%)	12 (4%)	0	100	100
1	B	336/338 (99%)	324 (96%)	12 (4%)	0	100	100
1	C	333/338 (98%)	324 (97%)	9 (3%)	0	100	100
1	D	330/338 (98%)	321 (97%)	9 (3%)	0	100	100
1	E	330/338 (98%)	317 (96%)	13 (4%)	0	100	100
1	F	336/338 (99%)	327 (97%)	9 (3%)	0	100	100
1	G	331/338 (98%)	321 (97%)	10 (3%)	0	100	100
1	H	333/338 (98%)	318 (96%)	15 (4%)	0	100	100
All	All	2657/2704 (98%)	2568 (97%)	89 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/282 (97%)	267 (97%)	7 (3%)	54	54
1	B	279/282 (99%)	273 (98%)	6 (2%)	60	62
1	C	278/282 (99%)	271 (98%)	7 (2%)	55	55
1	D	275/282 (98%)	268 (98%)	7 (2%)	55	55
1	E	278/282 (99%)	274 (99%)	4 (1%)	74	77
1	F	278/282 (99%)	268 (96%)	10 (4%)	42	39
1	G	278/282 (99%)	272 (98%)	6 (2%)	60	62
1	H	278/282 (99%)	267 (96%)	11 (4%)	38	33
All	All	2218/2256 (98%)	2160 (97%)	58 (3%)	54	54

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	84	ARG
1	A	142	ARG
1	A	176	ARG
1	A	275	PHE
1	A	297	TYR
1	A	301	GLU
1	B	18	ARG
1	B	138	SER
1	B	153	SER
1	B	226	LEU
1	B	275	PHE
1	B	286	ASN
1	C	11	ARG
1	C	24	ARG
1	C	33	THR
1	C	153	SER
1	C	166	GLU
1	C	178	ASP
1	C	275	PHE
1	D	8	GLU
1	D	23	ILE
1	D	30	ASN
1	D	142	ARG
1	D	153	SER
1	D	275	PHE
1	D	286	ASN
1	E	25	ASN
1	E	153	SER
1	E	213	ARG
1	E	275	PHE
1	F	18	ARG
1	F	85	ASP
1	F	153	SER
1	F	164	SER
1	F	202	GLU
1	F	213	ARG
1	F	236	SER
1	F	275	PHE
1	F	285	THR
1	F	335	GLU
1	G	30	ASN
1	G	85	ASP

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Mol	Chain	Res	Type
1	G	153	SER
1	G	205	ARG
1	G	236	SER
1	G	275	PHE
1	H	6	SER
1	H	25	ASN
1	H	29	ARG
1	H	131	ARG
1	H	153	SER
1	H	159	LEU
1	H	194	LEU
1	H	203	MET
1	H	226	LEU
1	H	275	PHE
1	H	286	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	231	GLN
1	B	41	ASN
1	B	200	ASN
1	C	74	ASN
1	E	12	ASN
1	E	25	ASN
1	E	74	ASN
1	E	200	ASN
1	F	12	ASN
1	F	25	ASN
1	F	307	HIS
1	F	338	ASN
1	G	74	ASN
1	G	129	GLN
1	G	200	ASN
1	H	25	ASN
1	H	227	GLN
1	H	286	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 22 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 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	332/338 (98%)	0.38	28 (8%) 14 14	29, 41, 60, 82	0
1	B	338/338 (100%)	0.44	30 (8%) 12 13	29, 44, 65, 78	0
1	C	335/338 (99%)	0.36	22 (6%) 22 22	25, 38, 60, 80	0
1	D	333/338 (98%)	0.33	25 (7%) 17 18	29, 39, 58, 81	0
1	E	333/338 (98%)	0.31	27 (8%) 15 15	25, 36, 56, 74	0
1	F	338/338 (100%)	0.41	28 (8%) 14 15	26, 40, 59, 68	0
1	G	335/338 (99%)	0.41	36 (10%) 8 8	28, 42, 63, 79	0
1	H	336/338 (99%)	0.43	33 (9%) 10 10	29, 41, 64, 80	0
2	K	17/17 (100%)	0.51	4 (23%) 1 1	30, 37, 89, 96	0
2	L	17/17 (100%)	0.49	4 (23%) 1 1	31, 38, 99, 103	0
2	M	17/17 (100%)	0.41	4 (23%) 1 1	29, 36, 86, 87	0
2	N	17/17 (100%)	0.48	4 (23%) 1 1	30, 36, 95, 95	0
2	O	17/17 (100%)	0.17	2 (11%) 6 6	29, 34, 93, 96	0
2	P	16/17 (94%)	0.10	1 (6%) 23 24	28, 37, 61, 78	0
2	Q	17/17 (100%)	0.32	3 (17%) 2 2	30, 38, 79, 82	0
2	R	17/17 (100%)	0.25	3 (17%) 2 2	29, 36, 89, 90	0
All	All	2815/2840 (99%)	0.38	254 (9%) 12 12	25, 40, 62, 103	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	28	VAL	7.6
1	H	28	VAL	7.3
1	G	28	VAL	6.9
1	H	26	ALA	6.5
1	B	28	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	285	THR	6.2
1	B	305	ALA	6.0
1	C	285	THR	5.8
1	B	339	GLY	5.7
1	C	305	ALA	5.6
1	G	26	ALA	5.6
1	F	339	GLY	5.4
1	E	285	THR	5.3
1	G	302	GLY	5.2
1	G	339	GLY	5.2
2	K	1	DA	5.1
1	A	304	SER	5.0
1	D	32	SER	5.0
1	H	27	PRO	5.0
1	A	305	ALA	4.9
1	F	285	THR	4.8
2	L	1	DA	4.7
1	C	284	GLY	4.7
1	G	27	PRO	4.7
1	D	302	GLY	4.6
1	C	28	VAL	4.6
1	D	304	SER	4.6
1	D	285	THR	4.5
1	D	305	ALA	4.5
1	E	25	ASN	4.5
1	A	177	LYS	4.4
1	C	339	GLY	4.3
2	O	1	DA	4.3
1	E	304	SER	4.2
1	F	12	ASN	4.2
1	G	178	ASP	4.2
1	D	284	GLY	4.2
1	G	285	THR	4.2
1	A	303	ARG	4.2
1	E	339	GLY	4.1
1	H	177	LYS	4.0
1	B	27	PRO	4.0
1	G	105	VAL	3.9
1	G	177	LYS	3.9
1	B	191	VAL	3.9
1	G	147	VAL	3.9
1	H	339	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	305	ALA	3.8
2	N	1	DA	3.8
1	A	302	GLY	3.8
1	D	339	GLY	3.7
1	H	336	LEU	3.7
1	B	26	ALA	3.6
1	C	336	LEU	3.6
1	A	11	ARG	3.6
1	B	338	ASN	3.6
1	B	147	VAL	3.5
1	G	284	GLY	3.5
1	C	11	ARG	3.4
1	C	304	SER	3.4
1	B	284	GLY	3.4
2	R	1	DA	3.4
1	C	338	ASN	3.4
1	F	336	LEU	3.4
1	D	177	LYS	3.4
1	F	113	CYS	3.4
2	M	1	DA	3.4
1	G	191	VAL	3.4
2	P	17	DT	3.4
2	Q	1	DA	3.3
2	O	2	DA	3.3
1	F	145	VAL	3.3
1	F	305	ALA	3.3
1	E	284	GLY	3.3
1	A	338	ASN	3.3
1	H	301	GLU	3.3
2	L	2	DA	3.2
1	H	178	ASP	3.2
1	A	189	LEU	3.2
1	E	336	LEU	3.2
1	E	113	CYS	3.2
1	H	239	VAL	3.2
1	B	189	LEU	3.2
1	C	26	ALA	3.2
1	G	108	ALA	3.2
2	N	2	DA	3.2
1	C	101	ILE	3.2
1	D	297[A]	TYR	3.2
1	F	26	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	145	VAL	3.1
1	C	109	VAL	3.1
1	H	131	ARG	3.1
1	H	302	GLY	3.1
1	E	109	VAL	3.0
1	G	11	ARG	3.0
1	H	25	ASN	3.0
2	N	3	DG	3.0
1	F	147	VAL	3.0
1	B	110	MET	3.0
2	K	17	DT	3.0
1	D	178	ASP	3.0
1	F	30	ASN	3.0
1	B	303	ARG	3.0
1	D	145	VAL	3.0
1	A	300	ALA	3.0
1	G	25	ASN	3.0
1	H	189	LEU	2.9
1	A	147	VAL	2.9
1	H	147	VAL	2.9
1	C	173	ALA	2.9
2	L	17	DT	2.9
1	D	336	LEU	2.9
1	F	146	ALA	2.9
2	N	17	DT	2.8
1	B	146	ALA	2.8
1	C	108	ALA	2.8
1	B	12	ASN	2.8
1	G	29	ARG	2.8
1	B	336	LEU	2.8
1	C	147	VAL	2.8
1	F	259	VAL	2.8
2	K	2	DA	2.8
1	F	85	ASP	2.8
1	C	178	ASP	2.7
1	F	114	ALA	2.7
1	E	147	VAL	2.7
1	A	32	SER	2.7
1	A	97	VAL	2.7
1	E	145	VAL	2.7
1	E	303	ARG	2.7
1	D	179	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	145	VAL	2.7
1	F	191	VAL	2.6
1	H	145	VAL	2.6
1	E	110	MET	2.6
1	B	109	VAL	2.6
1	H	146	ALA	2.6
1	D	114	ALA	2.6
1	G	176	ARG	2.6
1	A	285	THR	2.6
1	G	106	SER	2.6
1	E	191	VAL	2.6
1	D	338	ASN	2.6
1	H	30	ASN	2.6
1	G	30	ASN	2.6
1	H	192	VAL	2.6
1	B	85	ASP	2.6
1	D	30	ASN	2.5
1	F	25	ASN	2.5
1	F	177	LYS	2.5
2	M	2	DA	2.5
1	H	8	GLU	2.5
1	C	191	VAL	2.5
1	H	338	ASN	2.5
1	E	254	LEU	2.5
1	H	148	LEU	2.5
1	E	23	ILE	2.5
1	D	301	GLU	2.5
1	B	190	ALA	2.5
1	E	146	ALA	2.5
1	A	82	PHE	2.5
2	Q	17	DT	2.5
1	A	339	GLY	2.5
1	A	110	MET	2.4
1	H	297[A]	TYR	2.4
1	B	192	VAL	2.4
1	H	191	VAL	2.4
1	C	113	CYS	2.4
1	G	301	GLU	2.4
1	G	336	LEU	2.4
2	M	17	DT	2.4
1	B	107	SER	2.4
1	A	114	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	300	ALA	2.4
1	G	101	ILE	2.4
1	G	104	ILE	2.4
2	R	17	DT	2.4
1	E	114	ALA	2.4
1	D	101	ILE	2.4
1	A	129	GLN	2.4
1	A	113	CYS	2.4
1	F	82	PHE	2.4
1	G	15	THR	2.4
1	G	12	ASN	2.4
1	G	109	VAL	2.3
1	E	24	ARG	2.3
2	Q	2	DA	2.3
1	E	189	LEU	2.3
1	D	303	ARG	2.3
1	D	12	ASN	2.3
1	B	114	ALA	2.3
1	G	170	GLU	2.3
1	A	301	GLU	2.3
1	F	15	THR	2.3
1	E	305	ALA	2.3
1	G	114	ALA	2.3
1	H	32	SER	2.3
1	B	8	GLU	2.3
1	G	145	VAL	2.3
1	B	237	LEU	2.3
1	E	108	ALA	2.3
1	G	146	ALA	2.3
1	B	169	GLU	2.3
1	G	8	GLU	2.3
2	R	2	DA	2.3
1	E	8	GLU	2.3
2	K	3	DG	2.3
1	F	200	ASN	2.3
1	G	338	ASN	2.3
1	B	148	LEU	2.3
1	C	110	MET	2.2
1	H	180	LEU	2.2
1	G	110	MET	2.2
1	H	176	ARG	2.2
2	M	3	DG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	106	SER	2.2
1	G	107	SER	2.2
1	H	163	GLU	2.2
1	E	326	PHE	2.2
1	E	101	ILE	2.2
1	H	257	ALA	2.2
1	A	136	THR	2.2
1	E	259	VAL	2.2
1	H	105	VAL	2.2
1	F	27	PRO	2.2
1	B	113	CYS	2.1
1	F	107	SER	2.1
1	D	146	ALA	2.1
1	F	238	ALA	2.1
1	F	110	MET	2.1
1	A	336	LEU	2.1
1	F	163	GLU	2.1
1	F	202	GLU	2.1
1	H	29	ARG	2.1
1	A	178	ASP	2.1
1	H	283	GLU	2.1
1	D	11	ARG	2.1
1	G	297	TYR	2.1
1	B	145	VAL	2.1
1	D	147	VAL	2.1
1	E	239	VAL	2.1
2	L	3	DG	2.0
1	C	27	PRO	2.0
1	A	12	ASN	2.0
1	A	190	ALA	2.0
1	F	115	ALA	2.0
1	D	83	PHE	2.0
1	A	138	SER	2.0
1	A	254	LEU	2.0
1	H	107	SER	2.0
1	D	8	GLU	2.0
1	C	30	ASN	2.0
1	E	12	ASN	2.0
1	G	259	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	CA	E	340	1/1	0.99	0.19	1.38	34,34,34,34	0
3	CA	C	340	1/1	0.99	0.14	0.85	31,31,31,31	0
3	CA	D	341	1/1	0.98	0.14	0.49	42,42,42,42	0
3	CA	F	340	1/1	1.00	0.15	0.37	30,30,30,30	0
3	CA	A	1	1/1	0.99	0.15	0.35	31,31,31,31	0
3	CA	G	341	1/1	0.89	0.13	-0.01	48,48,48,48	0
3	CA	G	340	1/1	0.99	0.13	-0.12	34,34,34,34	0
3	CA	D	340	1/1	0.99	0.14	-0.18	29,29,29,29	0
3	CA	B	340	1/1	0.99	0.13	-0.21	33,33,33,33	0
3	CA	H	340	1/1	0.99	0.14	-0.28	33,33,33,33	0
3	CA	A	340	1/1	0.98	0.12	-0.84	45,45,45,45	0
3	CA	H	341	1/1	0.95	0.10	-1.22	43,43,43,43	0
3	CA	C	341	1/1	0.95	0.11	-1.40	43,43,43,43	0
3	CA	B	342	1/1	0.98	0.19	-	68,68,68,68	0
3	CA	D	342	1/1	0.85	0.10	-	66,66,66,66	0
3	CA	C	342	1/1	0.86	0.15	-	65,65,65,65	0
3	CA	F	342	1/1	0.82	0.09	-	68,68,68,68	0
3	CA	E	341	1/1	0.97	0.13	-	41,41,41,41	0
3	CA	A	341	1/1	0.94	0.11	-	77,77,77,77	0
3	CA	H	342	1/1	0.93	0.08	-	74,74,74,74	0
3	CA	B	341	1/1	0.97	0.17	-	48,48,48,48	0
3	CA	F	341	1/1	0.96	0.07	-	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.