Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 02:15 PM JST

PDB ID	:	8K27
EMDB ID	:	EMD-36830
Title	:	ICP1 Csy-dsDNA complex (partial duplex)
Authors	:	Zhang, L.X.; Feng, Y.
Deposited on	:	2023-07-12
Resolution	:	3.60 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

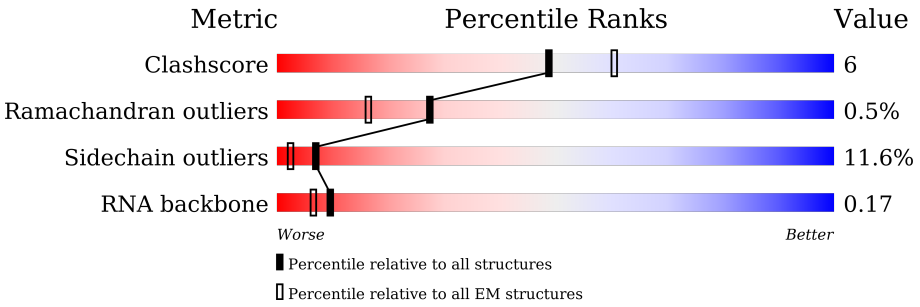
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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	179	79% 16% • •
2	B	248	81% 15% • •
3	C	306	87% 12% •
3	D	306	87% 11% •
3	E	306	91% 8% •
3	F	306	76% 19% • •
3	G	306	84% 15% •
3	H	306	66% 27% 5% •

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Mol	Chain	Length	Quality of chain
4	P	60	33% 55% 8%
5	Q	49	88% 12%
6	R	25	92% 8%
7	I	168	56% 34% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21183 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Csy1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	173	Total	C	N	O	S	0	0
			1382	876	230	266	10		

- Molecule 2 is a protein called Csy2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	246	Total	C	N	O	S	0	0
			1903	1215	319	355	14		

- Molecule 3 is a protein called Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	302	Total	C	N	O	S	0	0
			2305	1453	391	454	7		
3	C	302	Total	C	N	O	S	0	0
			2305	1453	391	454	7		
3	G	302	Total	C	N	O	S	0	0
			2305	1453	391	454	7		
3	F	302	Total	C	N	O	S	0	0
			2301	1450	390	454	7		
3	E	302	Total	C	N	O	S	0	0
			2305	1453	391	454	7		
3	H	302	Total	C	N	O	S	0	0
			2299	1450	388	454	7		

- Molecule 4 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	60	Total	C	N	O	P	0	0
			1260	565	210	425	60		

- Molecule 5 is a DNA chain called DNA (49-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	49	Total	C	N	O	P	0	0
			1013	482	193	289	49		

- Molecule 6 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	25	Total	C	N	O	P	0	0
			515	246	93	151	25		

- Molecule 7 is a protein called Csy4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	165	Total	C	N	O	S	0	0
			1290	818	221	245	6		

There is a discrepancy between the modelled and reference sequences:

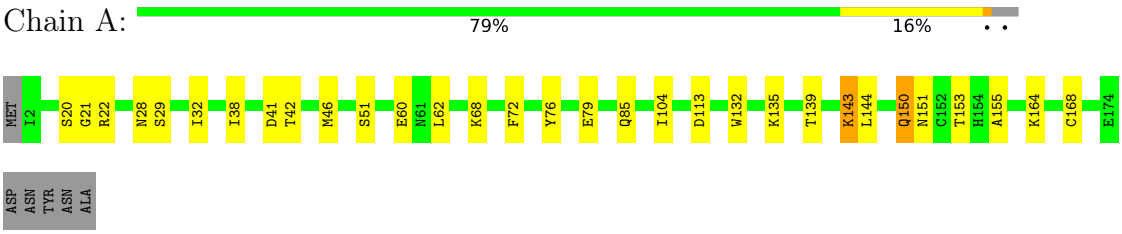
Chain	Residue	Modelled	Actual	Comment	Reference
I	51	ILE	VAL	conflict	UNP F1D5V5

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.

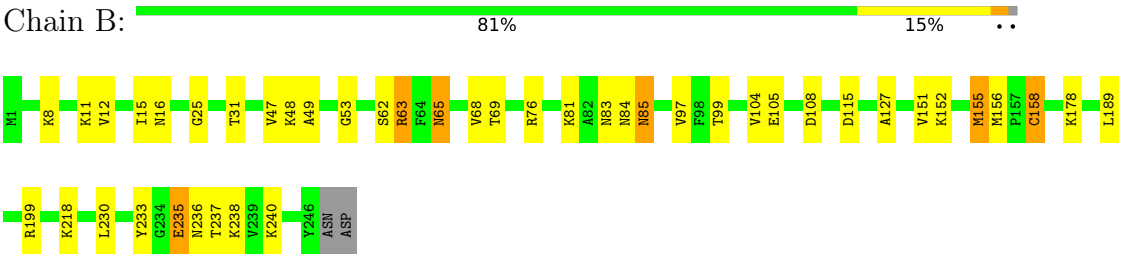
- Molecule 1: Csy1

Chain A:



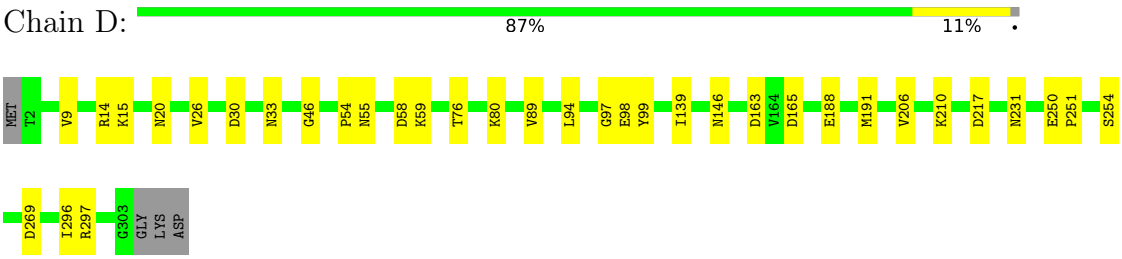
- Molecule 2: Csy2

Chain B:



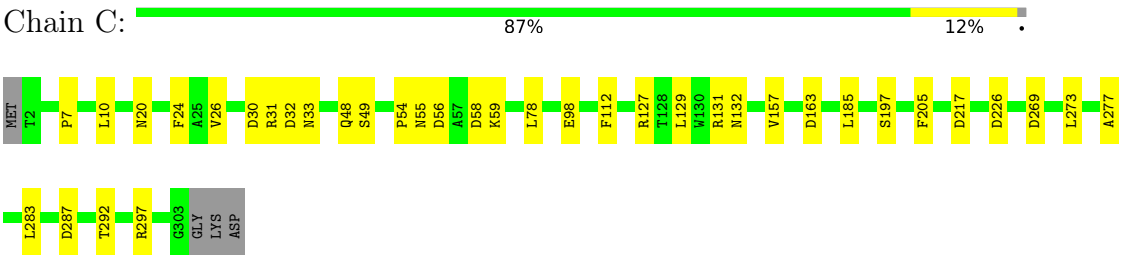
- Molecule 3: Csy3

Chain D:



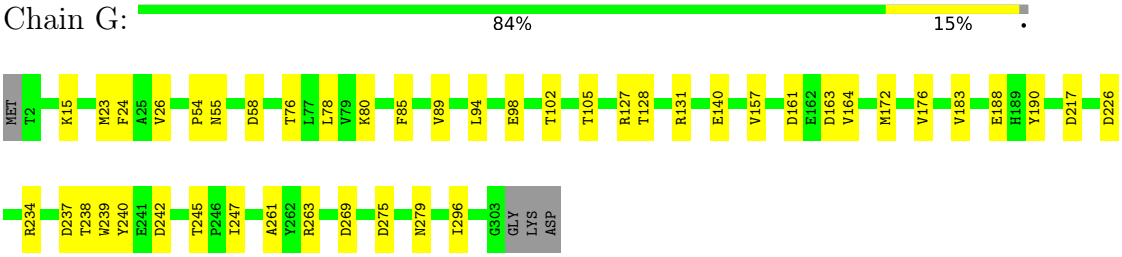
- Molecule 3: Csy3

Chain C:



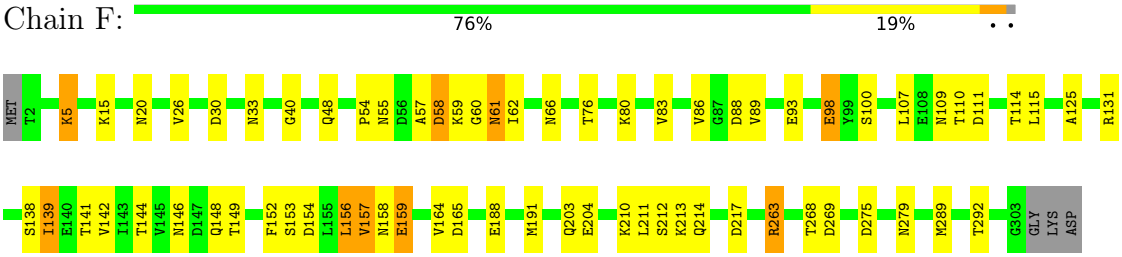
• Molecule 3: Csy3

Chain G:



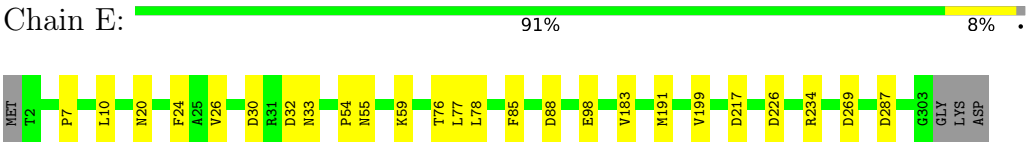
• Molecule 3: Csy3

Chain F:



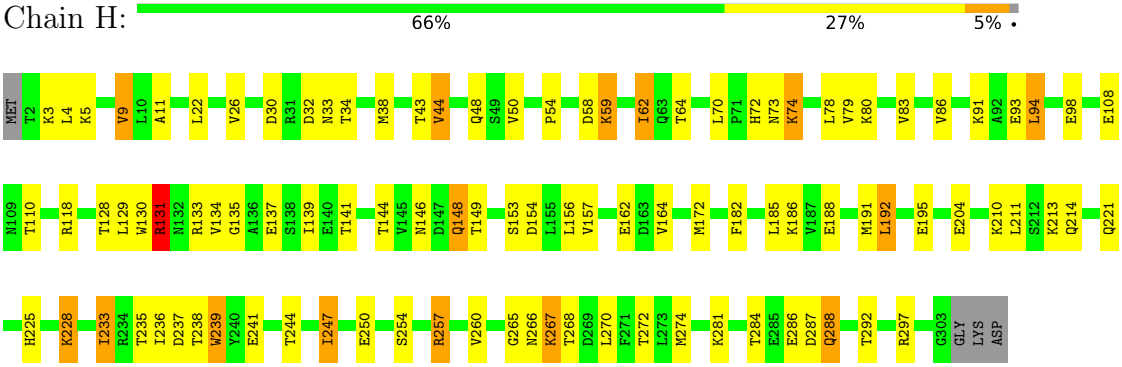
• Molecule 3: Csy3

Chain E:



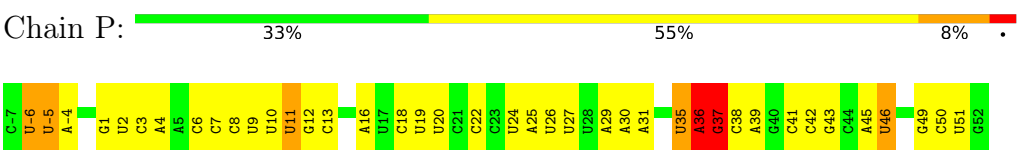
• Molecule 3: Csy3

Chain H:



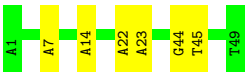
• Molecule 4: RNA (60-MER)

Chain P:



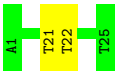
• Molecule 5: DNA (49-MER)

Chain Q:



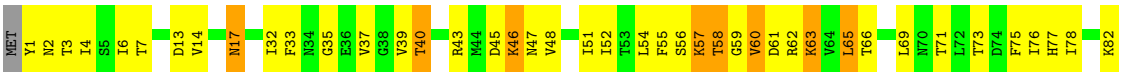
• Molecule 6: DNA (25-MER)

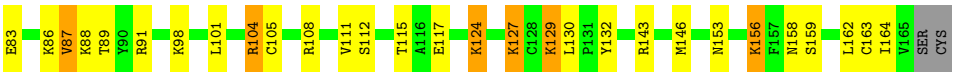
Chain R:



• Molecule 7: Csy4

Chain I:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	240070	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.27	0/1414	0.53	0/1909
2	B	0.28	0/1940	0.55	0/2623
3	C	0.28	0/2344	0.55	1/3183 (0.0%)
3	D	0.28	0/2344	0.56	1/3183 (0.0%)
3	E	0.29	0/2344	0.57	1/3183 (0.0%)
3	F	0.28	0/2340	0.53	1/3179 (0.0%)
3	G	0.27	0/2344	0.54	1/3183 (0.0%)
3	H	0.30	0/2338	0.56	1/3176 (0.0%)
4	P	0.56	2/1404 (0.1%)	1.27	4/2181 (0.2%)
5	Q	0.63	0/1139	0.96	0/1757
6	R	0.60	0/577	0.89	0/889
7	I	0.60	1/1308 (0.1%)	0.92	3/1757 (0.2%)
All	All	0.37	3/21836 (0.0%)	0.69	13/30203 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	36	A	O3'-P	-12.07	1.46	1.61
7	I	156	LYS	C-N	7.52	1.51	1.34
4	P	37	G	O3'-P	5.04	1.67	1.61

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	36	A	O3'-P-O5'	-37.71	32.35	104.00
4	P	36	A	P-O3'-C3'	-17.13	99.14	119.70
4	P	36	A	OP2-P-O3'	14.90	137.99	105.20
7	I	58	THR	O-C-N	12.46	144.38	123.20
7	I	58	THR	C-N-CA	-12.10	96.90	122.30
7	I	58	THR	CA-C-N	-11.07	94.06	116.20
4	P	36	A	OP1-P-O3'	-6.34	91.25	105.20
3	G	54	PRO	N-CA-CB	6.02	110.52	103.30
3	F	54	PRO	N-CA-CB	5.88	110.36	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	54	PRO	N-CA-CB	5.80	110.27	103.30
3	C	54	PRO	N-CA-CB	5.76	110.22	103.30
3	H	54	PRO	N-CA-CB	5.74	110.18	103.30
3	E	54	PRO	N-CA-CB	5.50	109.90	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1382	0	1327	16	0
2	B	1903	0	1925	18	0
3	C	2305	0	2239	14	0
3	D	2305	0	2239	16	0
3	E	2305	0	2239	14	0
3	F	2301	0	2228	21	0
3	G	2305	0	2239	22	0
3	H	2299	0	2228	32	0
4	P	1260	0	641	43	0
5	Q	1013	0	552	4	0
6	R	515	0	284	2	0
7	I	1290	0	1336	55	0
All	All	21183	0	19477	228	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 (228) 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)
7:I:4:ILE:HD13	7:I:65:LEU:HD21	1.15	1.09
7:I:6:ILE:HD11	7:I:65:LEU:CD1	1.82	1.08
7:I:4:ILE:CD1	7:I:65:LEU:HD21	1.88	1.01
4:P:36:A:C5	4:P:37:G:C5	2.52	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:4:ILE:HD13	7:I:65:LEU:CD2	1.97	0.95
4:P:36:A:C6	4:P:37:G:C6	2.56	0.93
4:P:36:A:C5	4:P:37:G:C6	2.62	0.87
7:I:61:ASP:HB2	7:I:63:LYS:NZ	1.91	0.85
7:I:6:ILE:HD11	7:I:65:LEU:HD13	1.59	0.85
4:P:36:A:H1'	4:P:37:G:O4'	1.77	0.84
7:I:6:ILE:HD11	7:I:65:LEU:HD12	1.59	0.84
3:H:131:ARG:HD3	7:I:14:VAL:HG12	1.60	0.82
4:P:36:A:C8	4:P:37:G:N7	2.48	0.80
4:P:36:A:C6	4:P:37:G:N1	2.50	0.80
3:F:26:VAL:O	3:F:76:THR:HB	1.80	0.79
7:I:61:ASP:O	7:I:65:LEU:HD23	1.83	0.77
4:P:36:A:C4	4:P:37:G:C4	2.74	0.74
3:H:131:ARG:CD	7:I:14:VAL:HG12	2.17	0.74
7:I:56:SER:HB3	7:I:60:VAL:HG22	1.70	0.73
3:G:26:VAL:O	3:G:76:THR:HB	1.90	0.72
4:P:35:U:H4'	4:P:36:A:H5'	1.72	0.71
2:B:62:SER:HB3	2:B:65:ASN:ND2	2.05	0.70
3:D:26:VAL:O	3:D:76:THR:HB	1.92	0.70
3:F:156:LEU:HD22	3:F:159:GLU:OE1	1.91	0.70
4:P:36:A:O2'	4:P:37:G:P	2.51	0.68
4:P:36:A:C8	4:P:37:G:C8	2.82	0.68
4:P:11:U:H5'	3:E:234:ARG:HH12	1.60	0.67
3:H:237:ASP:HB3	3:H:247:ILE:HG13	1.76	0.66
4:P:36:A:C4	4:P:37:G:C5	2.86	0.64
1:A:153:THR:HG22	1:A:155:ALA:H	1.64	0.63
7:I:6:ILE:CD1	7:I:65:LEU:CD1	2.70	0.63
4:P:36:A:N1	4:P:37:G:C2	2.67	0.63
7:I:61:ASP:HB2	7:I:63:LYS:HZ3	1.61	0.63
7:I:61:ASP:HB2	7:I:63:LYS:HZ2	1.65	0.62
4:P:36:A:N6	4:P:37:G:C6	2.68	0.62
7:I:40:THR:HB	7:I:55:PHE:HE2	1.65	0.61
3:H:48:GLN:OE1	3:H:50:VAL:HG23	2.00	0.60
7:I:3:THR:HB	7:I:55:PHE:HB3	1.84	0.59
4:P:36:A:N7	4:P:37:G:C5	2.69	0.59
3:D:15:LYS:HB2	3:D:296:ILE:HG23	1.85	0.59
3:E:77:LEU:HD13	3:E:199:VAL:HG11	1.84	0.59
3:E:287:ASP:OD1	3:E:287:ASP:N	2.35	0.58
7:I:7:THR:HB	7:I:77:HIS:HB3	1.85	0.58
4:P:36:A:O2'	4:P:37:G:H5"	2.04	0.57
4:P:36:A:N9	4:P:37:G:C8	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:NH2	1:A:151:ASN:O	2.38	0.56
4:P:36:A:C2	4:P:37:G:C2	2.93	0.56
3:H:131:ARG:HD3	7:I:14:VAL:CG1	2.33	0.56
3:C:129:LEU:HB3	3:C:132:ASN:HB2	1.87	0.56
4:P:37:G:H5'	4:P:38:C:H5'	1.87	0.56
1:A:41:ASP:OD1	1:A:41:ASP:N	2.38	0.56
3:D:30:ASP:OD2	3:D:33:ASN:ND2	2.39	0.56
3:G:237:ASP:HB3	3:G:247:ILE:HG13	1.87	0.56
7:I:57:LYS:C	7:I:59:GLY:N	2.56	0.56
4:P:36:A:H2	7:I:132:TYR:CZ	2.25	0.55
3:D:139:ILE:HG23	3:D:191:MET:HG2	1.90	0.54
3:E:85:PHE:HB2	3:E:183:VAL:HG12	1.90	0.54
3:H:110:THR:HG22	3:H:288:GLN:HG3	1.90	0.54
3:D:251:PRO:HG2	3:C:49:SER:HB3	1.90	0.54
3:G:127:ARG:NH2	3:G:157:VAL:O	2.41	0.53
3:F:48:GLN:HG2	3:F:60:GLY:HA2	1.90	0.53
4:P:24:U:OP2	3:G:234:ARG:NH2	2.41	0.53
3:F:80:LYS:HG2	3:F:188:GLU:HG2	1.91	0.53
3:H:267:LYS:HB3	3:H:272:THR:HG21	1.91	0.53
1:A:22:ARG:HD3	1:A:29:SER:H	1.74	0.52
3:E:76:THR:HA	3:E:191:MET:O	2.09	0.52
3:F:139:ILE:HG23	3:F:191:MET:HG2	1.91	0.52
7:I:73:THR:HA	7:I:76:ILE:HG22	1.91	0.52
1:A:32:ILE:HG21	2:B:189:LEU:HD23	1.90	0.52
7:I:111:VAL:HB	7:I:115:THR:HB	1.92	0.52
1:A:51:SER:O	1:A:51:SER:OG	2.27	0.52
3:H:130:TRP:CD1	7:I:13:ASP:OD1	2.62	0.52
3:H:48:GLN:HG3	3:H:59:LYS:HG3	1.92	0.51
4:P:50:C:H5"	7:I:164:ILE:HG23	1.91	0.51
2:B:199:ARG:NH2	4:P:-6:U:OP1	2.41	0.51
3:C:269:ASP:OD1	3:C:269:ASP:N	2.43	0.51
3:H:135:GLY:HA2	7:I:71:THR:HB	1.92	0.51
3:E:20:ASN:OD1	3:E:20:ASN:N	2.43	0.51
3:F:15:LYS:HE3	3:F:89:VAL:HA	1.92	0.50
3:G:102:THR:HA	3:G:105:THR:HG22	1.93	0.50
4:P:36:A:C1'	4:P:37:G:O4'	2.55	0.50
4:P:36:A:H1'	4:P:37:G:C8	2.47	0.50
3:D:20:ASN:N	3:D:20:ASN:OD1	2.44	0.50
4:P:39:A:H61	4:P:51:U:H3	1.59	0.50
1:A:60:GLU:OE2	1:A:68:LYS:NZ	2.45	0.50
4:P:36:A:C6	4:P:37:G:C2	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:36:A:N7	4:P:37:G:N7	2.60	0.49
7:I:101:LEU:HA	7:I:104:ARG:HB3	1.93	0.49
7:I:4:ILE:CG2	7:I:54:LEU:HB2	2.43	0.49
7:I:55:PHE:CD2	7:I:87:VAL:HG11	2.47	0.49
4:P:36:A:H1'	4:P:37:G:C5'	2.43	0.49
3:G:140:GLU:HB3	3:G:190:TYR:HB2	1.95	0.48
3:E:30:ASP:OD2	3:E:33:ASN:ND2	2.46	0.48
4:P:38:C:H2'	4:P:39:A:C8	2.48	0.48
5:Q:7:DA:N3	3:H:9:VAL:HG11	2.29	0.48
3:E:269:ASP:OD1	3:E:269:ASP:N	2.44	0.48
3:D:97:GLY:C	3:D:99:TYR:H	2.17	0.48
3:F:275:ASP:O	3:F:279:ASN:ND2	2.46	0.48
4:P:46:U:H4'	7:I:124:LYS:NZ	2.29	0.48
7:I:39:VAL:HG12	7:I:54:LEU:CD2	2.44	0.48
3:D:217:ASP:N	3:D:217:ASP:OD1	2.46	0.47
7:I:66:THR:HG22	7:I:78:ILE:HG13	1.96	0.47
2:B:47:VAL:HG22	2:B:104:VAL:HG12	1.95	0.47
3:C:163:ASP:N	3:C:163:ASP:OD1	2.47	0.47
3:C:217:ASP:OD1	3:C:217:ASP:N	2.47	0.47
3:H:239:TRP:CD1	3:H:286:GLU:HB2	2.49	0.47
7:I:40:THR:HB	7:I:55:PHE:CE2	2.47	0.47
4:P:27:U:OP1	3:G:131:ARG:NH1	2.48	0.47
4:P:36:A:C5	4:P:37:G:C4	2.99	0.47
4:P:36:A:H1'	4:P:37:G:H5"	1.96	0.47
3:C:24:PHE:HB2	3:C:78:LEU:HB3	1.96	0.47
3:F:110:THR:HG21	3:F:292:THR:OG1	2.14	0.47
3:E:217:ASP:OD1	3:E:217:ASP:N	2.47	0.47
2:B:155:MET:H	2:B:155:MET:HG3	1.47	0.47
3:H:130:TRP:NE1	7:I:13:ASP:OD1	2.47	0.47
4:P:36:A:C8	4:P:37:G:C5	3.02	0.47
3:C:226:ASP:N	3:C:226:ASP:OD1	2.48	0.47
7:I:4:ILE:O	7:I:54:LEU:N	2.48	0.47
3:E:24:PHE:HB2	3:E:78:LEU:HB3	1.97	0.47
7:I:129:LYS:HD3	7:I:129:LYS:HA	1.52	0.46
3:C:273:LEU:HD13	3:C:287:ASP:HB2	1.98	0.46
7:I:3:THR:CB	7:I:55:PHE:HB3	2.45	0.46
2:B:218:LYS:HD3	2:B:218:LYS:HA	1.75	0.46
3:H:204:GLU:HG2	3:H:214:GLN:HB3	1.96	0.46
1:A:72:PHE:O	1:A:76:TYR:HB2	2.15	0.46
4:P:43:G:H2'	4:P:45:A:H2	1.79	0.46
3:G:261:ALA:HB2	3:F:57:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:74:LYS:HB2	3:H:74:LYS:HE2	1.46	0.46
3:C:127:ARG:NH2	3:C:157:VAL:O	2.49	0.46
3:C:277:ALA:HB2	3:C:283:LEU:HD11	1.97	0.46
3:C:112:PHE:HE1	3:C:292:THR:HG21	1.80	0.46
3:H:233:ILE:H	3:H:233:ILE:HG12	1.60	0.46
4:P:3:C:OP1	3:C:131:ARG:NH1	2.50	0.45
1:A:143:LYS:H	1:A:143:LYS:HG2	1.52	0.45
2:B:235:GLU:H	2:B:235:GLU:HG2	1.40	0.45
3:D:269:ASP:OD1	3:D:269:ASP:N	2.47	0.45
3:G:176:VAL:HG21	3:G:183:VAL:HB	1.99	0.45
7:I:158:ASN:HB2	7:I:159:SER:H	1.62	0.45
2:B:49:ALA:HB1	2:B:230:LEU:HD12	1.97	0.45
3:F:269:ASP:OD1	3:F:269:ASP:N	2.49	0.45
3:H:93:GLU:H	3:H:93:GLU:HG2	1.55	0.45
7:I:7:THR:O	7:I:77:HIS:N	2.45	0.45
3:G:24:PHE:HB2	3:G:78:LEU:HB3	1.98	0.45
3:G:275:ASP:O	3:G:279:ASN:ND2	2.46	0.45
7:I:89:THR:HG21	7:I:153:ASN:HA	1.98	0.45
2:B:11:LYS:HG2	2:B:97:VAL:HG22	1.99	0.45
6:R:22:DT:H6	6:R:22:DT:H2'	1.58	0.45
3:G:240:TYR:HB3	3:G:263:ARG:HE	1.82	0.45
3:G:217:ASP:OD1	3:G:217:ASP:N	2.50	0.44
3:F:217:ASP:N	3:F:217:ASP:OD1	2.50	0.44
7:I:2:ASN:HA	7:I:83:GLU:HA	1.98	0.44
7:I:57:LYS:H	7:I:57:LYS:HG2	1.39	0.44
3:F:263:ARG:HG3	3:F:268:THR:HG23	1.99	0.44
2:B:31:THR:HG21	2:B:127:ALA:HB2	1.99	0.44
3:D:14:ARG:HG3	4:P:4:A:H5"	1.98	0.44
3:G:85:PHE:HB2	3:G:183:VAL:HG12	2.00	0.44
3:F:5:LYS:HA	3:F:5:LYS:HD3	1.46	0.44
3:F:125:ALA:HB1	3:F:157:VAL:HA	1.99	0.44
3:D:46:GLY:HA3	4:P:11:U:H1'	1.99	0.44
2:B:48:LYS:HE3	2:B:48:LYS:HB2	1.71	0.44
3:F:48:GLN:HB3	3:F:61:ASN:HD21	1.82	0.44
3:H:11:ALA:HB3	3:H:94:LEU:HB2	1.99	0.44
1:A:38:ILE:HD12	1:A:42:THR:HB	2.00	0.44
3:H:148:GLN:HE21	3:H:148:GLN:HB2	1.58	0.44
3:H:133:ARG:NH1	7:I:13:ASP:OD2	2.51	0.43
7:I:33:PHE:HD1	7:I:37:VAL:O	2.01	0.43
4:P:11:U:H4'	3:E:234:ARG:HH22	1.83	0.43
3:G:128:THR:O	3:G:128:THR:OG1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:127:LYS:HD2	7:I:127:LYS:HA	1.68	0.43
3:G:296:ILE:HD13	3:G:296:ILE:HA	1.91	0.43
3:G:23:MET:HA	3:G:78:LEU:O	2.17	0.43
3:G:15:LYS:HD2	3:G:89:VAL:HA	2.00	0.43
7:I:39:VAL:HG12	7:I:54:LEU:HD23	2.01	0.43
1:A:168:CYS:HB2	2:B:25:GLY:HA3	2.00	0.43
5:Q:14:DA:H5"	3:E:59:LYS:HE3	2.01	0.43
3:H:131:ARG:CD	7:I:14:VAL:CG1	2.92	0.43
5:Q:22:DA:H2'	5:Q:23:DA:C8	2.53	0.43
3:H:62:ILE:H	3:H:62:ILE:HG13	1.58	0.43
1:A:20:SER:OG	1:A:21:GLY:N	2.51	0.43
3:D:250:GLU:OE2	3:D:254:SER:OG	2.28	0.43
4:P:36:A:N6	4:P:37:G:N1	2.65	0.43
3:F:159:GLU:H	3:F:159:GLU:HG3	1.52	0.43
2:B:16:ASN:OD1	2:B:16:ASN:N	2.48	0.43
7:I:37:VAL:HG22	7:I:56:SER:HB2	2.01	0.43
3:H:118:ARG:HB3	3:H:236:ILE:HG21	2.00	0.42
7:I:124:LYS:HA	7:I:124:LYS:HD3	1.34	0.42
1:A:104:ILE:HD13	4:P:-5:U:H5"	2.01	0.42
3:H:129:LEU:H	3:H:129:LEU:HG	1.52	0.42
3:H:228:LYS:HB3	3:H:228:LYS:HE3	1.25	0.42
2:B:8:LYS:HA	2:B:99:THR:HG22	2.01	0.42
2:B:12:VAL:HB	2:B:15:ILE:HD11	2.02	0.42
2:B:62:SER:HB3	2:B:65:ASN:HD22	1.82	0.42
5:Q:44:DG:H2'	5:Q:45:DT:H71	2.01	0.42
3:G:58:ASP:N	3:G:58:ASP:OD1	2.50	0.42
3:F:115:LEU:HD21	3:F:289:MET:HB3	2.01	0.42
3:G:55:ASN:OD1	3:G:55:ASN:N	2.53	0.42
7:I:17:ASN:ND2	7:I:47:ASN:HB3	2.35	0.42
3:H:137:GLU:HB2	3:H:192:LEU:HB3	2.01	0.42
2:B:62:SER:OG	2:B:63:ARG:N	2.52	0.41
3:D:9:VAL:HB	3:D:94:LEU:HD23	2.02	0.41
3:C:20:ASN:OD1	3:C:20:ASN:N	2.51	0.41
3:H:131:ARG:NE	7:I:14:VAL:HG12	2.35	0.41
3:D:163:ASP:OD1	3:D:163:ASP:N	2.54	0.41
3:G:269:ASP:N	3:G:269:ASP:OD1	2.54	0.41
3:H:257:ARG:H	3:H:257:ARG:HG2	1.64	0.41
7:I:46:LYS:H	7:I:46:LYS:HG2	1.40	0.41
1:A:139:THR:HG21	1:A:164:LYS:HD3	2.02	0.41
6:R:21:DT:H6	6:R:21:DT:H2'	1.75	0.41
3:G:80:LYS:HG2	3:G:188:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:40:GLY:O	3:F:66:ASN:ND2	2.42	0.41
3:F:110:THR:HG21	3:F:292:THR:CB	2.51	0.41
3:H:58:ASP:OD1	3:H:58:ASP:N	2.54	0.41
3:H:130:TRP:HD1	7:I:13:ASP:HB3	1.85	0.41
3:E:26:VAL:O	3:E:76:THR:HB	2.21	0.41
3:C:7:PRO:HD2	3:C:10:LEU:HD11	2.03	0.41
3:E:7:PRO:HD2	3:E:10:LEU:HD11	2.03	0.41
3:H:22:LEU:HD23	3:H:22:LEU:HA	1.92	0.41
3:F:15:LYS:HG3	3:F:89:VAL:HG12	2.02	0.40
2:B:53:GLY:HA3	2:B:158:CYS:SG	2.61	0.40
3:D:80:LYS:HG2	3:D:188:GLU:HG2	2.03	0.40
3:H:131:ARG:CZ	7:I:14:VAL:HG12	2.52	0.40
7:I:164:ILE:HD13	7:I:164:ILE:HG21	1.62	0.40
3:D:15:LYS:HD2	3:D:89:VAL:HA	2.02	0.40
3:F:30:ASP:OD2	3:F:33:ASN:ND2	2.55	0.40
1:A:46:MET:HE1	1:A:62:LEU:HB3	2.02	0.40
1:A:150:GLN:H	1:A:150:GLN:HG2	1.60	0.40
7:I:104:ARG:NH1	7:I:108:ARG:HD2	2.36	0.40
4:P:36:A:C2	4:P:37:G:N3	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	171/179 (96%)	161 (94%)	10 (6%)	0	100 100
2	B	244/248 (98%)	225 (92%)	17 (7%)	2 (1%)	16 51
3	C	300/306 (98%)	279 (93%)	21 (7%)	0	100 100
3	D	300/306 (98%)	286 (95%)	14 (5%)	0	100 100
3	E	300/306 (98%)	282 (94%)	18 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	F	300/306 (98%)	274 (91%)	24 (8%)	2 (1%)	19 53
3	G	300/306 (98%)	278 (93%)	22 (7%)	0	100 100
3	H	300/306 (98%)	258 (86%)	37 (12%)	5 (2%)	7 37
7	I	163/168 (97%)	149 (91%)	11 (7%)	3 (2%)	7 35
All	All	2378/2431 (98%)	2192 (92%)	174 (7%)	12 (0%)	27 59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	85	ASN
3	H	43	THR
3	H	44	VAL
2	B	233	TYR
3	H	59	LYS
7	I	32	ILE
7	I	35	GLY
3	F	98	GLU
7	I	98	LYS
3	H	131	ARG
3	F	58	ASP
3	H	265	GLY

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 PDB entries followed by that with respect to all EM entries.

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	152/157 (97%)	143 (94%)	9 (6%)	16 45
2	B	209/211 (99%)	186 (89%)	23 (11%)	5 25
3	C	242/251 (96%)	227 (94%)	15 (6%)	15 44
3	D	242/251 (96%)	232 (96%)	10 (4%)	26 55
3	E	242/251 (96%)	237 (98%)	5 (2%)	48 71
3	F	241/251 (96%)	198 (82%)	43 (18%)	1 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	G	242/251 (96%)	231 (96%)	11 (4%)	23 53
3	H	241/251 (96%)	164 (68%)	77 (32%)	0 1
7	I	148/151 (98%)	113 (76%)	35 (24%)	0 4
All	All	1959/2025 (97%)	1731 (88%)	228 (12%)	7 23

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	79	GLU
1	A	85	GLN
1	A	113	ASP
1	A	132	TRP
1	A	135	LYS
1	A	143	LYS
1	A	144	LEU
1	A	150	GLN
2	B	63	ARG
2	B	65	ASN
2	B	68	VAL
2	B	69	THR
2	B	76	ARG
2	B	81	LYS
2	B	83	ASN
2	B	84	ASN
2	B	85	ASN
2	B	105	GLU
2	B	108	ASP
2	B	115	ASP
2	B	151	VAL
2	B	152	LYS
2	B	155	MET
2	B	156	MET
2	B	158	CYS
2	B	178	LYS
2	B	235	GLU
2	B	236	ASN
2	B	237	THR
2	B	238	LYS
2	B	240	LYS
3	D	55	ASN

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Mol	Chain	Res	Type
3	D	58	ASP
3	D	59	LYS
3	D	98	GLU
3	D	146	ASN
3	D	165	ASP
3	D	206	VAL
3	D	210	LYS
3	D	231	ASN
3	D	297	ARG
3	C	26	VAL
3	C	30	ASP
3	C	31	ARG
3	C	32	ASP
3	C	33	ASN
3	C	48	GLN
3	C	55	ASN
3	C	56	ASP
3	C	58	ASP
3	C	59	LYS
3	C	98	GLU
3	C	185	LEU
3	C	197	SER
3	C	205	PHE
3	C	297	ARG
3	G	94	LEU
3	G	98	GLU
3	G	161	ASP
3	G	163	ASP
3	G	164	VAL
3	G	172	MET
3	G	226	ASP
3	G	238	THR
3	G	239	TRP
3	G	242	ASP
3	G	245	THR
3	F	5	LYS
3	F	20	ASN
3	F	55	ASN
3	F	58	ASP
3	F	59	LYS
3	F	61	ASN
3	F	62	ILE

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Mol	Chain	Res	Type
3	F	83	VAL
3	F	86	VAL
3	F	88	ASP
3	F	93	GLU
3	F	98	GLU
3	F	100	SER
3	F	107	LEU
3	F	109	ASN
3	F	111	ASP
3	F	114	THR
3	F	131	ARG
3	F	138	SER
3	F	139	ILE
3	F	141	THR
3	F	142	VAL
3	F	144	THR
3	F	146	ASN
3	F	148	GLN
3	F	149	THR
3	F	152	PHE
3	F	153	SER
3	F	154	ASP
3	F	156	LEU
3	F	157	VAL
3	F	158	ASN
3	F	159	GLU
3	F	164	VAL
3	F	165	ASP
3	F	203	GLN
3	F	204	GLU
3	F	210	LYS
3	F	211	LEU
3	F	212	SER
3	F	213	LYS
3	F	214	GLN
3	F	263	ARG
3	E	32	ASP
3	E	55	ASN
3	E	88	ASP
3	E	98	GLU
3	E	226	ASP
3	H	3	LYS

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Mol	Chain	Res	Type
3	H	4	LEU
3	H	5	LYS
3	H	9	VAL
3	H	26	VAL
3	H	30	ASP
3	H	32	ASP
3	H	33	ASN
3	H	34	THR
3	H	38	MET
3	H	44	VAL
3	H	62	ILE
3	H	64	THR
3	H	70	LEU
3	H	72	HIS
3	H	73	ASN
3	H	74	LYS
3	H	78	LEU
3	H	79	VAL
3	H	80	LYS
3	H	83	VAL
3	H	86	VAL
3	H	91	LYS
3	H	94	LEU
3	H	98	GLU
3	H	108	GLU
3	H	128	THR
3	H	131	ARG
3	H	134	VAL
3	H	139	ILE
3	H	141	THR
3	H	144	THR
3	H	146	ASN
3	H	148	GLN
3	H	149	THR
3	H	153	SER
3	H	154	ASP
3	H	156	LEU
3	H	157	VAL
3	H	162	GLU
3	H	164	VAL
3	H	172	MET
3	H	182	PHE

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Mol	Chain	Res	Type
3	H	185	LEU
3	H	186	LYS
3	H	188	GLU
3	H	191	MET
3	H	192	LEU
3	H	195	GLU
3	H	210	LYS
3	H	211	LEU
3	H	213	LYS
3	H	221	GLN
3	H	225	HIS
3	H	228	LYS
3	H	233	ILE
3	H	235	THR
3	H	238	THR
3	H	239	TRP
3	H	241	GLU
3	H	244	THR
3	H	247	ILE
3	H	250	GLU
3	H	254	SER
3	H	257	ARG
3	H	260	VAL
3	H	266	ASN
3	H	267	LYS
3	H	268	THR
3	H	270	LEU
3	H	274	MET
3	H	281	LYS
3	H	284	THR
3	H	287	ASP
3	H	288	GLN
3	H	292	THR
3	H	297	ARG
7	I	1	TYR
7	I	17	ASN
7	I	40	THR
7	I	43	ARG
7	I	45	ASP
7	I	46	LYS
7	I	48	VAL
7	I	51	ILE

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Mol	Chain	Res	Type
7	I	52	ILE
7	I	57	LYS
7	I	58	THR
7	I	60	VAL
7	I	62	ARG
7	I	63	LYS
7	I	65	LEU
7	I	69	LEU
7	I	75	PHE
7	I	82	LYS
7	I	86	LYS
7	I	87	VAL
7	I	88	LYS
7	I	91	ARG
7	I	104	ARG
7	I	105	CYS
7	I	112	SER
7	I	117	GLU
7	I	124	LYS
7	I	127	LYS
7	I	129	LYS
7	I	130	LEU
7	I	143	ARG
7	I	146	MET
7	I	156	LYS
7	I	162	LEU
7	I	163	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	65	ASN
3	D	33	ASN
3	D	231	ASN
3	F	61	ASN
3	H	66	ASN
3	H	73	ASN
3	H	148	GLN
3	H	266	ASN
3	H	288	GLN
3	H	294	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	P	59/60 (98%)	30 (50%)	3 (5%)

All (30) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	P	-6	U
4	P	-5	U
4	P	-4	A
4	P	1	G
4	P	2	U
4	P	6	C
4	P	7	C
4	P	8	C
4	P	9	U
4	P	10	U
4	P	11	U
4	P	12	G
4	P	13	C
4	P	16	A
4	P	18	C
4	P	19	U
4	P	20	U
4	P	22	C
4	P	25	A
4	P	26	U
4	P	29	A
4	P	30	A
4	P	31	A
4	P	35	U
4	P	36	A
4	P	37	G
4	P	41	C
4	P	42	C
4	P	46	U
4	P	49	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	P	35	U
4	P	36	A

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Mol	Chain	Res	Type
4	P	41	C

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)

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.