



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 07:12 PM UTC

PDB ID : 8EDG / pdb_00008edg
EMDB ID : EMD-28034
Title : Cryo-EM structure of the Hermes transposase bound to two left-ends of its DNA transposon
Authors : Lannes, L.; Dyda, F.
Deposited on : 2022-09-04
Resolution : 4.64 Å (reported)
Based on initial models : 8EB5, 6DX0, 4D1Q

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 : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

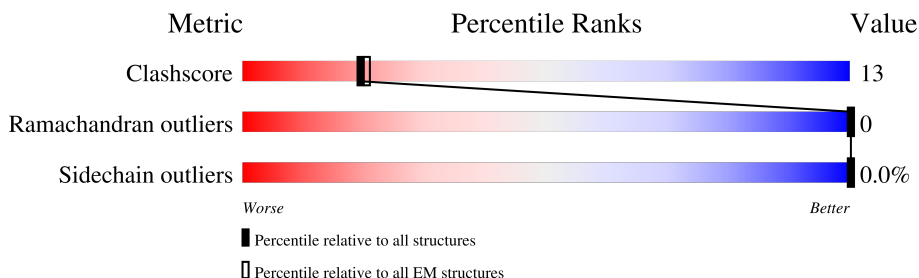
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.64 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	M	7	43% 57%
1	P	7	14% 86%
2	N	46	37% 63%
2	Q	46	57% 43%
3	O	55	53% 47%
3	R	55	73% 27%
4	A	612	59% 31% 10%
4	C	612	67% 23% 10%
4	E	612	64% 26% 10%

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Mol	Chain	Length	Quality of chain
4	G	612	60% 30% 10%
4	I	612	9% • 88%
4	K	612	8% • 88%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23358 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 DNA chain called DNA (5'-D(*GP*CP*GP*TP*GP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	7	Total	C	N	O	P	0	0
			144	69	30	39	6		
1	P	7	Total	C	N	O	P	0	0
			144	69	30	39	6		

- Molecule 2 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	46	Total	C	N	O	P	0	0
			941	451	173	272	45		
2	Q	46	Total	C	N	O	P	0	0
			941	451	173	272	45		

- Molecule 3 is a DNA chain called DNA (55-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	55	Total	C	N	O	P	0	0
			1126	538	200	333	55		
3	R	55	Total	C	N	O	P	0	0
			1126	538	200	333	55		

- Molecule 4 is a protein called Hermes transposase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	550	Total	C	N	O	S	0	0
			4432	2830	757	820	25		
4	C	550	Total	C	N	O	S	0	0
			4432	2830	757	820	25		
4	I	74	Total	C	N	O	S	0	0
			601	379	108	108	6		
4	E	550	Total	C	N	O	S	0	0
			4432	2830	757	820	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	550	Total	C	N	O	S	0	0
			4432	2830	757	820	25		
4	K	74	Total	C	N	O	S	0	0
			601	379	108	108	6		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	GLN	engineered mutation	UNP Q25438
A	128	GLY	LYS	engineered mutation	UNP Q25438
C	2	GLU	GLN	engineered mutation	UNP Q25438
C	128	GLY	LYS	engineered mutation	UNP Q25438
I	2	GLU	GLN	engineered mutation	UNP Q25438
I	128	GLY	LYS	engineered mutation	UNP Q25438
E	2	GLU	GLN	engineered mutation	UNP Q25438
E	128	GLY	LYS	engineered mutation	UNP Q25438
G	2	GLU	GLN	engineered mutation	UNP Q25438
G	128	GLY	LYS	engineered mutation	UNP Q25438
K	2	GLU	GLN	engineered mutation	UNP Q25438
K	128	GLY	LYS	engineered mutation	UNP Q25438

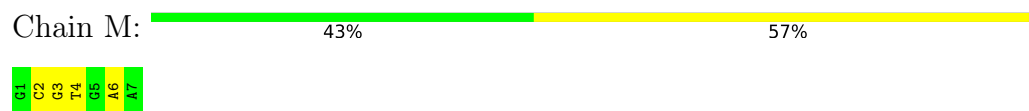
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	G	1	Total	Zn	0
			1	1	
5	K	1	Total	Zn	0
			1	1	

3 Residue-property plots

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.

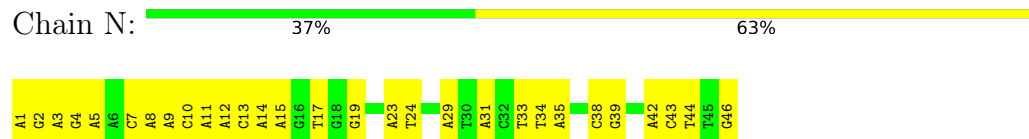
- Molecule 1: DNA (5'-D(*GP*CP*GP*TP*GP*AP*A)-3')



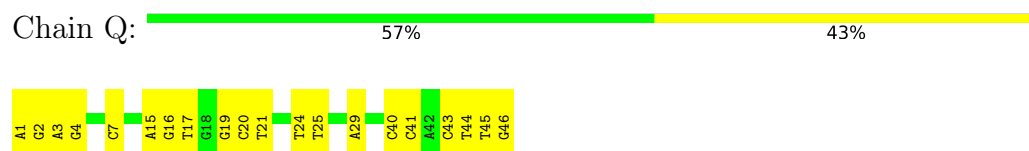
- Molecule 1: DNA (5'-D(*GP*CP*GP*TP*GP*AP*A)-3')



- Molecule 2: DNA (46-MER)



- Molecule 2: DNA (46-MER)

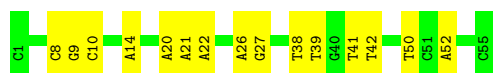


- Molecule 3: DNA (55-MER)



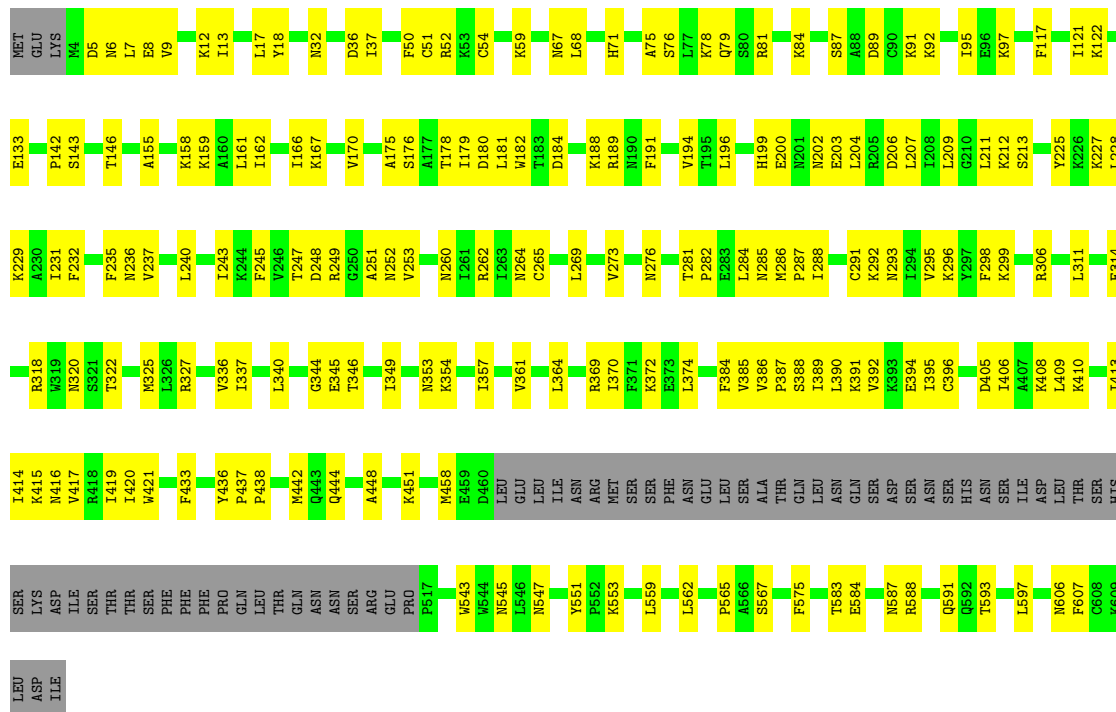
- Molecule 3: DNA (55-MER)





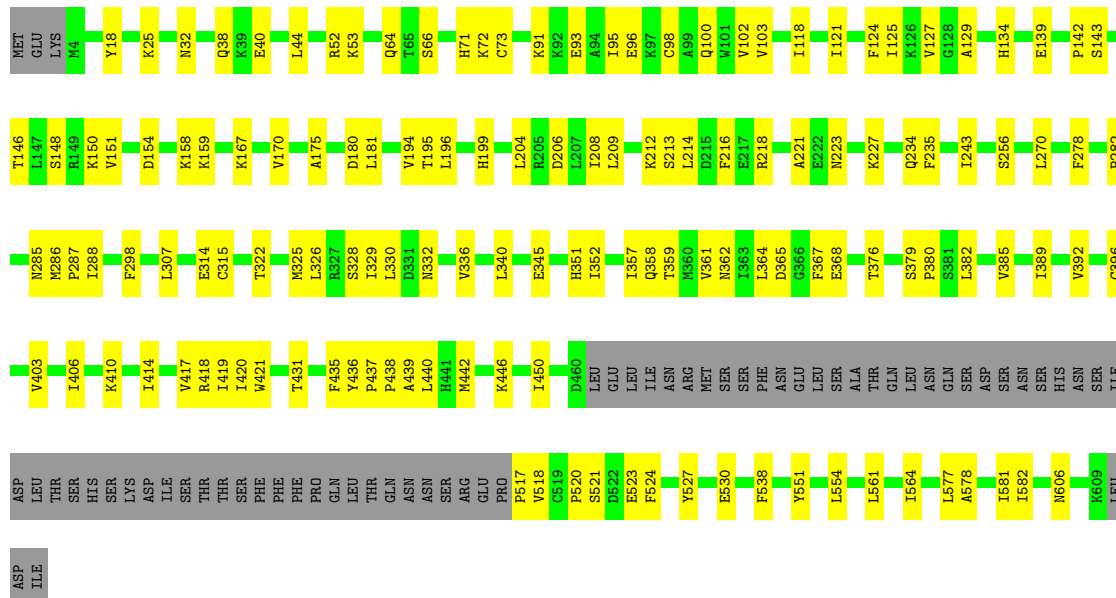
• Molecule 4: Hermes transposase

Chain A: 59% 31% 10%



• Molecule 4: Hermes transposase

Chain C: 67% 23% 10%



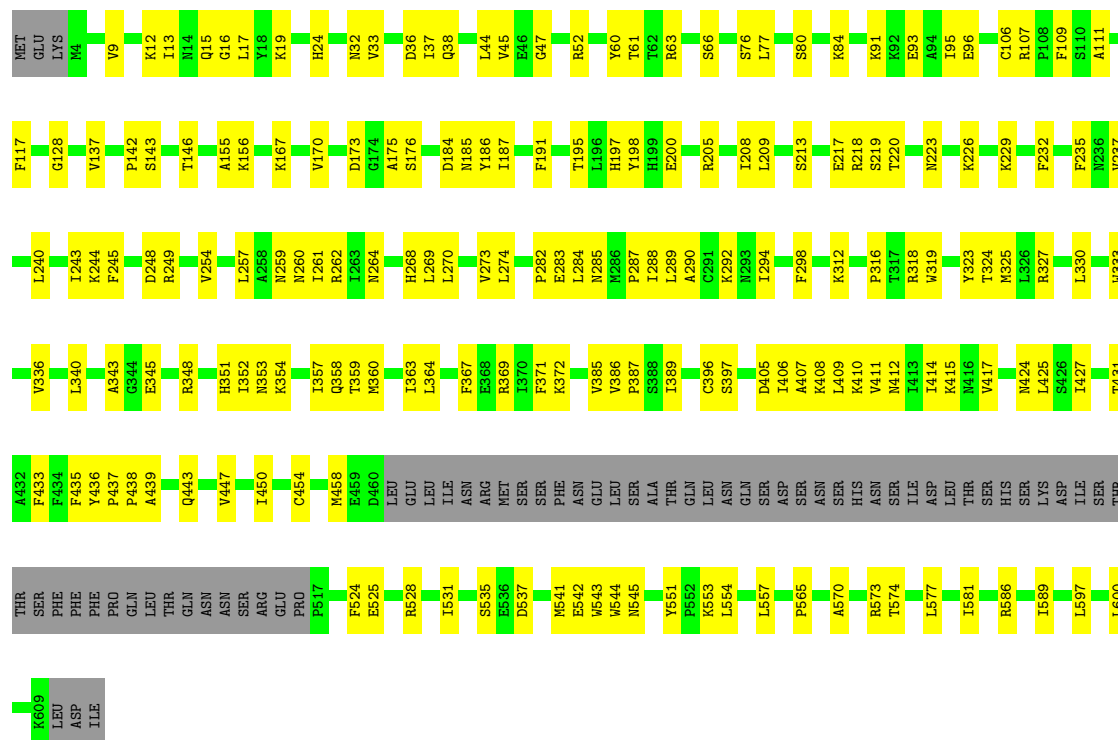
Chain I: 9% . 88%

Chain E: 64% 26% 10%



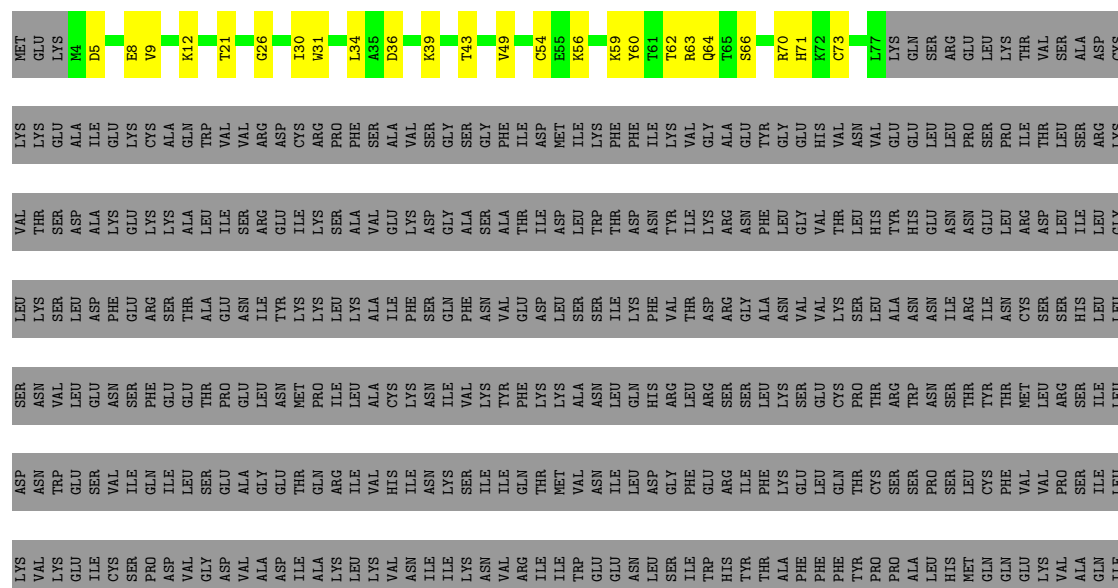
• Molecule 4: Hermes transposase

Chain G: 60% 30% 10%



• Molecule 4: Hermes transposase

Chain K: 8% 88%



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22.3	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

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: ZN

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	M	0.07	0/162	0.19	0/249
1	P	0.16	0/162	0.32	0/249
2	N	0.17	0/1056	0.33	0/1628
2	Q	0.17	0/1056	0.36	0/1628
3	O	0.16	0/1261	0.33	0/1944
3	R	0.18	0/1261	0.36	0/1944
4	A	0.13	0/4516	0.39	0/6089
4	C	0.13	0/4516	0.36	0/6089
4	E	0.14	0/4516	0.37	0/6089
4	G	0.12	0/4516	0.35	0/6089
4	I	0.11	0/611	0.30	0/821
4	K	0.12	0/611	0.31	0/821
All	All	0.14	0/24244	0.36	0/33640

There are no bond length outliers.

There are no bond angle outliers.

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	M	144	0	80	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	144	0	80	6	0
2	N	941	0	521	25	0
2	Q	941	0	521	16	0
3	O	1126	0	623	23	0
3	R	1126	0	623	13	0
4	A	4432	0	4513	143	0
4	C	4432	0	4513	97	0
4	E	4432	0	4513	112	0
4	G	4432	0	4513	134	0
4	I	601	0	611	11	0
4	K	601	0	611	15	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
All	All	23358	0	21722	551	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 13.

All (551) 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)
4:E:54:CYS:HB3	4:E:73:CYS:SG	2.05	0.96
4:A:385:VAL:HB	4:A:433:PHE:HZ	1.37	0.90
4:A:51:CYS:SG	4:A:54:CYS:HB3	2.13	0.86
4:G:357:ILE:HA	4:G:360:MET:HE2	1.59	0.82
4:A:51:CYS:SG	4:A:54:CYS:CB	2.67	0.82
3:O:45:DC:H5''	4:A:318:ARG:HH12	1.45	0.81
4:C:212:LYS:HE3	4:C:227:LYS:HE2	1.65	0.78
4:G:354:LYS:HB3	4:G:358:GLN:HE22	1.49	0.77
4:E:49:VAL:HG13	4:E:60:TYR:HB2	1.68	0.76
4:G:173:ASP:O	4:G:244:LYS:NZ	2.20	0.75
4:A:75:ALA:HB1	4:A:79:GLN:HE22	1.50	0.74
3:R:9:DG:H2''	3:R:10:DC:H2'	1.70	0.73
4:I:21:THR:HB	4:I:36:ASP:HB3	1.70	0.73
2:N:12:DA:H2''	2:N:13:DC:H5''	1.69	0.73
4:G:248:ASP:OD1	4:G:268:HIS:ND1	2.22	0.73
4:A:448:ALA:HA	4:A:451:LYS:HD3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:29:DA:OP1	4:C:72:LYS:NZ	2.22	0.72
4:C:287:PRO:HB3	4:C:352:ILE:HG12	1.71	0.71
4:E:96:GLU:O	4:E:100:GLN:NE2	2.23	0.71
4:A:340:LEU:HD12	4:A:345:GLU:HB2	1.73	0.70
4:G:289:LEU:HD23	4:G:292:LYS:HZ3	1.56	0.70
4:A:194:VAL:HG23	4:A:209:LEU:HB2	1.74	0.69
4:C:32:ASN:O	4:C:52:ARG:NH2	2.25	0.69
4:E:286:MET:SD	4:E:287:PRO:HD3	2.33	0.69
4:C:288:ILE:HD11	4:C:325:MET:HE3	1.73	0.69
4:C:382:LEU:HD22	4:C:564:ILE:HB	1.75	0.68
2:Q:21:DT:O4	4:K:64:GLN:NE2	2.27	0.68
4:A:75:ALA:O	4:A:79:GLN:NE2	2.27	0.68
4:K:71:HIS:HD2	4:K:73:CYS:SG	2.12	0.68
4:G:312:LYS:H	4:G:325:MET:HE1	1.58	0.67
4:A:276:ASN:HB3	4:A:416:ASN:HD21	1.60	0.67
4:A:337:ILE:HG12	4:A:349:ILE:HD12	1.76	0.67
4:G:37:ILE:HG23	4:G:45:VAL:HB	1.77	0.67
4:A:597:LEU:HD13	4:C:103:VAL:HG23	1.77	0.67
2:N:23:DA:H2''	2:N:24:DT:H5'	1.77	0.66
4:G:24:HIS:ND1	4:G:36:ASP:OD1	2.29	0.66
4:C:439:ALA:HA	4:C:442:MET:HE3	1.78	0.66
4:A:265:CYS:SG	4:A:567:SER:OG	2.53	0.66
4:C:206:ASP:O	4:C:606:ASN:ND2	2.29	0.66
4:I:51:CYS:SG	4:I:52:ARG:N	2.68	0.65
2:N:29:DA:OP1	4:E:56:LYS:NZ	2.29	0.65
4:E:107:ARG:HH22	4:G:111:ALA:HA	1.61	0.65
4:G:319:TRP:HB3	4:G:371:PHE:HE2	1.62	0.65
4:G:76:SER:O	4:G:80:SER:OG	2.14	0.65
4:E:282:PRO:HA	4:E:285:ASN:HB2	1.79	0.64
4:E:6:ASN:HD21	4:E:48:TRP:CD1	2.15	0.64
4:G:232:PHE:HB3	4:G:237:VAL:HB	1.80	0.64
4:A:240:LEU:HD13	4:A:243:ILE:HG13	1.80	0.64
4:A:282:PRO:HA	4:A:285:ASN:HB2	1.79	0.64
4:E:13:ILE:HG22	4:E:18:TYR:HB2	1.80	0.64
2:Q:19:DG:H2''	2:Q:20:DC:H5'	1.78	0.64
4:A:295:VAL:HG12	4:A:311:LEU:HD13	1.79	0.64
4:E:150:LYS:HE2	4:G:95:ILE:HG12	1.80	0.64
4:C:577:LEU:O	4:C:581:ILE:HD12	1.98	0.63
4:G:324:THR:HA	4:G:327:ARG:HE	1.62	0.63
4:A:51:CYS:SG	4:A:54:CYS:HB2	2.38	0.63
4:C:194:VAL:HG23	4:C:209:LEU:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:551:TYR:HB3	4:G:554:LEU:HB3	1.80	0.63
4:E:447:VAL:HA	4:E:450:ILE:HG22	1.80	0.63
3:R:14:DA:N6	4:C:64:GLN:OE1	2.31	0.62
4:C:195:THR:HG22	4:C:208:ILE:HG22	1.81	0.62
4:C:170:VAL:HG23	4:C:243:ILE:HD11	1.81	0.62
3:O:9:DG:H2''	3:O:10:DC:H5''	1.81	0.62
4:E:195:THR:HA	4:E:208:ILE:HA	1.81	0.62
4:G:323:TYR:CZ	4:G:327:ARG:HD3	2.34	0.62
4:G:458:MET:HE2	4:G:557:LEU:HD22	1.81	0.62
4:A:167:LYS:NZ	4:A:236:ASN:O	2.27	0.62
4:A:292:LYS:HD2	4:A:314:GLU:HG3	1.80	0.62
1:P:5:DG:H2''	1:P:6:DA:C8	2.35	0.62
4:C:71:HIS:CD2	4:C:73:CYS:HB3	2.33	0.62
4:G:287:PRO:HG3	4:G:352:ILE:HG12	1.82	0.62
4:G:244:LYS:HG3	4:G:261:ILE:HD11	1.82	0.61
4:A:87:SER:OG	4:A:89:ASP:OD1	2.18	0.61
4:G:270:LEU:HD23	4:G:371:PHE:HE1	1.64	0.61
4:A:54:CYS:SG	4:A:71:HIS:CE1	2.93	0.61
4:A:176:SER:HB3	4:A:565:PRO:HD3	1.81	0.61
4:E:316:PRO:HG2	4:E:318:ARG:HB2	1.82	0.61
4:G:405:ASP:HA	4:G:408:LYS:HE3	1.82	0.61
4:A:200:GLU:HB2	4:A:203:GLU:HG2	1.82	0.60
4:C:167:LYS:NZ	4:C:235:PHE:O	2.34	0.60
3:R:41:DT:H2''	3:R:42:DT:H5'	1.81	0.60
3:R:52:DA:N6	1:P:3:DG:O6	2.34	0.60
4:K:66:SER:OG	4:K:70:ARG:NH1	2.35	0.60
4:C:328:SER:O	4:C:332:ASN:ND2	2.34	0.60
4:G:541:MET:SD	4:G:545:ASN:ND2	2.71	0.60
2:N:33:DT:H2''	2:N:34:DT:H5'	1.84	0.60
2:N:2:DG:N1	3:O:46:DT:O2	2.34	0.60
3:O:35:DT:H2''	3:O:36:DT:C5	2.37	0.59
4:A:91:LYS:NZ	4:C:139:GLU:O	2.36	0.59
4:A:95:ILE:HG22	4:C:142:PRO:HG3	1.83	0.59
4:G:217:GLU:OE2	4:G:223:ASN:ND2	2.33	0.59
1:M:3:DG:H2''	1:M:4:DT:H5'	1.82	0.59
4:A:320:ASN:HD21	4:A:364:LEU:HD12	1.68	0.59
4:C:167:LYS:HA	4:C:170:VAL:HG12	1.85	0.59
4:C:446:LYS:O	4:C:450:ILE:HG12	2.03	0.59
4:E:23:ARG:HD3	4:E:24:HIS:H	1.66	0.59
4:E:248:ASP:O	4:E:262:ARG:NH2	2.36	0.59
3:O:2:DA:OP1	4:E:573:ARG:NH1	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:95:ILE:HG22	4:G:142:PRO:HG3	1.86	0.58
3:O:8:DC:H2''	3:O:9:DG:H5'	1.85	0.58
4:E:122:LYS:HG2	4:G:137:VAL:HG21	1.85	0.58
4:E:449:GLN:HB3	4:E:453:PHE:CE2	2.39	0.58
2:Q:17:DT:OP1	4:K:56:LYS:NZ	2.35	0.58
4:A:200:GLU:N	4:A:203:GLU:O	2.34	0.58
4:A:202:ASN:ND2	4:A:545:ASN:OD1	2.37	0.58
4:E:159:LYS:HB3	4:E:235:PHE:HE1	1.69	0.57
4:K:34:LEU:HG	4:K:49:VAL:HG11	1.86	0.57
4:E:67:ASN:OD1	4:E:70:ARG:NH2	2.36	0.57
4:E:248:ASP:OD2	4:E:249:ARG:NE	2.35	0.57
4:E:367:PHE:HA	4:E:370:ILE:HD12	1.84	0.57
2:N:43:DC:H4'	2:N:44:DT:H5'	1.85	0.57
4:A:384:PHE:HA	4:A:387:PRO:HG2	1.85	0.57
4:C:551:TYR:HB3	4:C:554:LEU:HB3	1.86	0.57
4:E:608:CYS:SG	4:E:609:LYS:N	2.73	0.57
4:E:308:ARG:HG2	4:E:332:ASN:HD21	1.69	0.57
4:A:385:VAL:HB	4:A:433:PHE:CZ	2.27	0.57
4:G:325:MET:HA	4:G:325:MET:HE3	1.87	0.57
4:G:340:LEU:HD12	4:G:345:GLU:HB2	1.87	0.57
4:E:150:LYS:NZ	4:G:95:ILE:HG23	2.20	0.56
4:C:326:LEU:HD13	4:C:329:ILE:HD11	1.86	0.56
4:G:412:ASN:HA	4:G:415:LYS:HZ3	1.69	0.56
4:K:8:GLU:HG2	4:K:12:LYS:HE2	1.87	0.56
4:A:281:THR:HG21	4:A:409:LEU:HD23	1.87	0.56
4:C:358:GLN:O	4:C:362:ASN:ND2	2.38	0.56
4:E:158:LYS:O	4:E:162:ILE:HG12	2.05	0.56
4:E:162:ILE:O	4:E:166:ILE:HD12	2.06	0.56
4:A:180:ASP:OD1	4:A:181:LEU:N	2.39	0.56
4:A:265:CYS:HG	4:A:567:SER:HG	1.53	0.56
2:N:42:DA:H2''	2:N:43:DC:O5'	2.04	0.56
4:A:84:LYS:N	4:C:134:HIS:O	2.35	0.55
4:I:39:LYS:NZ	4:I:44:LEU:O	2.39	0.55
2:N:9:DA:H2''	2:N:10:DC:H5''	1.87	0.55
4:G:259:ASN:ND2	4:G:260:ASN:OD1	2.40	0.55
4:A:269:LEU:HB3	4:A:421:TRP:CD1	2.42	0.55
4:A:391:LYS:O	4:A:395:ILE:HG12	2.06	0.55
4:G:38:GLN:HG3	4:G:44:LEU:HD13	1.88	0.55
4:E:39:LYS:HZ2	4:E:45:VAL:HA	1.71	0.55
4:A:386:VAL:HA	4:A:389:ILE:HG12	1.88	0.55
4:A:583:THR:HG22	4:A:584:GLU:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:458:MET:HB3	4:G:553:LYS:NZ	2.22	0.55
4:A:419:ILE:HG23	4:A:420:ILE:HG23	1.88	0.54
4:E:39:LYS:NZ	4:E:45:VAL:HA	2.23	0.54
4:E:552:PRO:HG2	4:E:553:LYS:HZ2	1.72	0.54
4:G:170:VAL:HG21	4:G:237:VAL:HG22	1.90	0.54
4:G:458:MET:HB3	4:G:553:LYS:HZ3	1.70	0.54
2:N:33:DT:O4	4:E:64:GLN:NE2	2.40	0.54
4:E:431:THR:HG22	4:E:450:ILE:HG13	1.88	0.54
4:C:204:LEU:HD11	4:C:380:PRO:HD3	1.88	0.54
4:E:247:THR:O	4:E:262:ARG:NH2	2.40	0.54
4:A:232:PHE:HB3	4:A:237:VAL:HB	1.90	0.54
4:A:406:ILE:HG22	4:A:410:LYS:HD2	1.89	0.54
4:G:175:ALA:HB3	4:G:243:ILE:HG22	1.88	0.54
4:A:353:ASN:OD1	4:A:354:LYS:N	2.40	0.54
4:A:296:LYS:HA	4:A:299:LYS:HG2	1.90	0.54
3:R:38:DT:H2''	3:R:39:DT:H5'	1.89	0.54
4:E:91:LYS:O	4:E:95:ILE:HG23	2.09	0.54
4:E:427:ILE:HA	4:E:430:TYR:HD2	1.73	0.53
4:E:583:THR:HG23	4:E:585:LYS:H	1.73	0.53
4:A:162:ILE:O	4:A:166:ILE:HD12	2.08	0.53
4:C:286:MET:HE1	4:C:351:HIS:HB3	1.90	0.53
4:G:323:TYR:HB2	4:G:364:LEU:HD13	1.90	0.53
4:A:357:ILE:O	4:A:361:VAL:HG23	2.09	0.53
4:G:439:ALA:H	4:G:531:ILE:HG22	1.72	0.53
4:A:6:ASN:OD1	4:A:7:LEU:N	2.42	0.53
4:C:91:LYS:O	4:C:95:ILE:HG12	2.08	0.53
4:C:431:THR:HG22	4:C:450:ILE:HD12	1.91	0.53
4:C:124:PHE:HA	4:C:127:VAL:HG12	1.90	0.53
4:G:195:THR:HA	4:G:208:ILE:HA	1.90	0.53
3:O:30:DA:H2''	3:O:31:DC:H5'	1.91	0.52
4:A:158:LYS:O	4:A:162:ILE:HG12	2.10	0.52
4:E:38:GLN:OE1	4:E:38:GLN:N	2.42	0.52
1:P:6:DA:H2''	1:P:7:DA:H5''	1.92	0.52
4:C:167:LYS:O	4:C:170:VAL:N	2.41	0.52
4:G:176:SER:OG	4:G:197:HIS:O	2.27	0.52
4:G:285:ASN:HA	4:G:288:ILE:HD12	1.91	0.52
2:Q:2:DG:H2''	2:Q:3:DA:H5''	1.91	0.52
4:A:196:LEU:HB2	4:A:209:LEU:HD11	1.90	0.52
4:G:61:THR:HG22	4:G:63:ARG:HG2	1.91	0.52
4:K:59:LYS:NZ	4:K:60:TYR:O	2.42	0.52
4:G:385:VAL:O	4:G:389:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:52:DA:OP1	4:G:218:ARG:NH1	2.43	0.52
4:E:220:THR:HG23	4:E:223:ASN:H	1.74	0.52
4:E:416:ASN:O	4:E:420:ILE:HB	2.10	0.52
2:Q:2:DG:OP1	4:G:573:ARG:NH2	2.39	0.52
3:O:15:DG:H2''	3:O:16:DT:H5'	1.91	0.52
4:I:31:TRP:HA	4:I:34:LEU:HB3	1.91	0.52
4:C:270:LEU:HD13	4:C:421:TRP:HZ3	1.76	0.51
4:G:9:VAL:O	4:G:13:ILE:HG12	2.11	0.51
4:K:30:ILE:HG23	4:K:31:TRP:CD1	2.46	0.51
2:Q:44:DT:H3'	2:Q:45:DT:H71	1.92	0.51
2:N:14:DA:H2''	2:N:15:DA:C8	2.45	0.51
4:G:359:THR:O	4:G:363:ILE:HG12	2.11	0.51
3:R:9:DG:H4'	3:R:10:DC:OP1	2.11	0.51
2:Q:43:DC:H2''	2:Q:44:DT:H5''	1.92	0.51
4:C:359:THR:HA	4:C:362:ASN:HD21	1.75	0.51
4:G:240:LEU:O	4:G:260:ASN:ND2	2.39	0.51
4:A:288:ILE:O	4:A:292:LYS:HG2	2.10	0.51
4:C:414:ILE:HG12	4:C:418:ARG:HH12	1.76	0.51
4:E:144:PRO:HB3	4:G:109:PHE:HB3	1.94	0.50
4:C:221:ALA:HA	4:C:256:SER:HB3	1.91	0.50
4:I:63:ARG:HG3	4:I:64:GLN:HG2	1.93	0.50
4:E:189:ARG:HD3	4:E:216:PHE:HE2	1.76	0.50
4:E:382:LEU:HD22	4:E:564:ILE:HB	1.93	0.50
3:O:19:DC:H1'	3:O:20:DA:C8	2.46	0.50
4:A:184:ASP:OD1	4:A:188:LYS:N	2.42	0.50
4:C:365:ASP:O	4:C:368:GLU:HG3	2.11	0.50
3:R:8:DC:H2''	3:R:9:DG:O4'	2.11	0.50
4:G:184:ASP:OD2	4:G:187:ILE:N	2.42	0.50
4:G:436:TYR:HD1	4:G:437:PRO:HD2	1.75	0.50
4:K:62:THR:OG1	4:K:63:ARG:NH1	2.42	0.50
4:A:117:PHE:O	4:A:121:ILE:HG12	2.11	0.50
4:C:340:LEU:HD22	4:C:345:GLU:HB2	1.93	0.50
4:E:33:VAL:O	4:E:52:ARG:NE	2.44	0.50
2:N:1:DA:H2''	2:N:2:DG:H5''	1.94	0.50
4:E:308:ARG:HG2	4:E:332:ASN:ND2	2.25	0.50
4:G:282:PRO:HA	4:G:285:ASN:HB2	1.92	0.50
4:G:330:LEU:HD21	4:G:357:ILE:HG21	1.93	0.50
4:A:159:LYS:HD2	4:A:235:PHE:HE1	1.76	0.50
3:O:5:DT:H4'	4:G:589:ILE:HD13	1.93	0.49
2:Q:1:DA:H4'	4:G:573:ARG:HH21	1.76	0.49
4:C:159:LYS:NZ	4:C:234:GLN:OE1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:403:VAL:HG12	4:E:406:ILE:HG13	1.93	0.49
4:G:289:LEU:HA	4:G:292:LYS:HG2	1.93	0.49
4:E:37:ILE:HD11	4:E:50:PHE:HB2	1.94	0.49
4:A:248:ASP:O	4:A:262:ARG:NH1	2.46	0.49
4:A:269:LEU:HB3	4:A:421:TRP:HD1	1.78	0.49
4:E:176:SER:HA	4:E:244:LYS:HB2	1.94	0.49
4:G:298:PHE:HZ	4:G:336:VAL:HG23	1.77	0.49
4:G:535:SER:OG	4:G:537:ASP:OD1	2.26	0.49
2:Q:40:DC:H2''	2:Q:41:DC:H5'	1.93	0.49
4:A:121:ILE:HD12	4:C:124:PHE:CD2	2.48	0.49
4:A:143:SER:O	4:A:146:THR:OG1	2.25	0.49
4:C:180:ASP:OD1	4:C:181:LEU:N	2.46	0.49
4:I:10:LYS:HE2	4:I:57:VAL:HG22	1.95	0.49
4:E:197:HIS:NE2	4:E:206:ASP:OD1	2.43	0.49
4:G:396:CYS:HA	4:G:410:LYS:HE2	1.94	0.49
3:R:20:DA:H2''	3:R:21:DA:C8	2.48	0.49
4:E:23:ARG:NH2	4:E:32:ASN:OD1	2.46	0.49
4:G:167:LYS:HA	4:G:170:VAL:HG22	1.94	0.49
4:G:439:ALA:O	4:G:443:GLN:NE2	2.32	0.49
4:C:175:ALA:HB1	4:C:196:LEU:HD11	1.94	0.49
4:G:245:PHE:HE2	4:G:260:ASN:HD22	1.60	0.49
1:M:6:DA:OP1	4:A:249:ARG:NH2	2.45	0.49
4:G:209:LEU:HD12	4:G:235:PHE:CD2	2.48	0.49
4:G:577:LEU:O	4:G:581:ILE:HG12	2.13	0.49
4:A:182:TRP:HB2	4:A:575:PHE:CZ	2.47	0.48
4:A:420:ILE:HG13	4:A:421:TRP:N	2.28	0.48
4:E:180:ASP:OD1	4:E:181:LEU:N	2.46	0.48
4:G:32:ASN:O	4:G:52:ARG:NH2	2.45	0.48
2:N:17:DT:OP1	4:I:56:LYS:NZ	2.33	0.48
4:C:121:ILE:O	4:C:125:ILE:HG12	2.13	0.48
4:E:287:PRO:HB3	4:E:352:ILE:HG12	1.94	0.48
4:E:383:CYS:SG	4:E:384:PHE:N	2.86	0.48
3:O:31:DC:H2''	3:O:32:DT:H72	1.95	0.48
4:G:354:LYS:O	4:G:358:GLN:NE2	2.47	0.48
4:A:191:PHE:HB3	4:A:211:LEU:HD11	1.94	0.48
4:G:348:ARG:HA	4:G:351:HIS:CE1	2.48	0.48
4:K:21:THR:HB	4:K:36:ASP:HB3	1.95	0.48
4:C:96:GLU:O	4:C:100:GLN:HG2	2.14	0.48
4:E:8:GLU:O	4:E:12:LYS:HG2	2.12	0.48
2:N:10:DC:H2''	2:N:11:DA:H5'	1.96	0.48
4:E:525:GLU:HB3	4:E:529:LYS:HZ2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:220:THR:HG23	4:G:223:ASN:H	1.77	0.48
2:N:46:DG:H2'	4:E:318:ARG:HH12	1.78	0.48
4:A:340:LEU:O	4:A:344:GLY:N	2.44	0.48
4:C:53:LYS:HE3	4:C:73:CYS:SG	2.54	0.48
4:E:123:PHE:CE1	4:G:93:GLU:HG3	2.49	0.48
4:G:412:ASN:HA	4:G:415:LYS:NZ	2.29	0.48
4:A:92:LYS:HA	4:A:92:LYS:HD2	1.76	0.48
4:C:18:TYR:HE1	4:C:40:GLU:HG3	1.78	0.48
4:E:118:ILE:HA	4:E:121:ILE:HG12	1.96	0.48
2:N:3:DA:H2''	2:N:4:DG:H8	1.79	0.47
4:A:32:ASN:O	4:A:52:ARG:NH2	2.47	0.47
4:A:158:LYS:HD2	4:A:161:LEU:HD12	1.96	0.47
4:A:458:MET:SD	4:A:553:LYS:HB3	2.54	0.47
4:A:391:LYS:O	4:A:394:GLU:HG3	2.15	0.47
4:C:389:ILE:HA	4:C:392:VAL:HG22	1.96	0.47
4:G:436:TYR:CD1	4:G:438:PRO:HD2	2.49	0.47
2:N:8:DA:H2''	2:N:9:DA:C8	2.49	0.47
4:C:521:SER:HA	4:C:524:PHE:CD2	2.49	0.47
4:A:262:ARG:HH12	4:A:264:ASN:HA	1.78	0.47
4:I:53:LYS:HB3	4:I:73:CYS:SG	2.54	0.47
4:G:454:CYS:O	4:G:458:MET:HG2	2.14	0.47
3:O:8:DC:H2''	3:O:9:DG:H2'	1.96	0.47
4:A:178:THR:O	4:A:179:ILE:HD13	2.14	0.47
4:C:143:SER:O	4:C:146:THR:OG1	2.28	0.47
4:C:199:HIS:ND1	4:C:204:LEU:HA	2.30	0.47
4:C:419:ILE:HG13	4:C:420:ILE:HG13	1.95	0.47
2:Q:15:DA:H4'	2:Q:16:DG:OP1	2.14	0.47
1:P:2:DC:H2''	1:P:3:DG:C8	2.50	0.47
4:A:285:ASN:HA	4:A:288:ILE:HD12	1.97	0.47
4:A:414:ILE:HA	4:A:417:VAL:HG22	1.96	0.47
4:A:437:PRO:HB2	4:A:438:PRO:HD3	1.96	0.47
2:Q:24:DT:H4'	2:Q:25:DT:H5'	1.97	0.47
4:A:245:PHE:HE2	4:A:260:ASN:HD22	1.62	0.47
4:C:278:PHE:HZ	4:C:288:ILE:HG21	1.79	0.47
4:E:178:THR:OG1	4:E:246:VAL:O	2.29	0.47
4:G:191:PHE:CE1	4:G:213:SER:HB3	2.50	0.47
4:G:437:PRO:HG3	4:G:543:TRP:CZ3	2.50	0.47
4:G:525:GLU:HA	4:G:528:ARG:HD3	1.96	0.47
4:A:76:SER:HA	4:A:81:ARG:HH22	1.79	0.47
4:I:71:HIS:CD2	4:I:73:CYS:HB2	2.50	0.47
2:Q:45:DT:H2'	2:Q:46:DG:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:196:LEU:HB3	4:A:207:LEU:HB3	1.96	0.47
4:E:199:HIS:HB2	4:E:204:LEU:HD23	1.97	0.47
4:G:333:TRP:HA	4:G:336:VAL:HG12	1.97	0.47
4:A:179:ILE:HD12	4:A:194:VAL:HG12	1.97	0.47
4:G:323:TYR:O	4:G:327:ARG:HG3	2.15	0.47
4:A:206:ASP:O	4:A:606:ASN:ND2	2.41	0.46
4:A:298:PHE:CZ	4:A:336:VAL:HG23	2.50	0.46
4:E:284:LEU:C	4:E:287:PRO:HD2	2.40	0.46
4:G:218:ARG:NH1	4:G:219:SER:O	2.44	0.46
4:G:340:LEU:HD13	4:G:343:ALA:HB3	1.96	0.46
4:K:54:CYS:SG	4:K:56:LYS:HG2	2.55	0.46
2:N:38:DC:H2''	2:N:39:DG:H5'	1.96	0.46
4:E:48:TRP:HD1	4:E:59:LYS:HA	1.80	0.46
4:K:71:HIS:CD2	4:K:73:CYS:H	2.33	0.46
4:A:410:LYS:HA	4:A:413:ILE:HG12	1.97	0.46
4:A:293:ASN:HA	4:A:296:LYS:HG2	1.97	0.46
4:G:283:GLU:H	4:G:283:GLU:CD	2.23	0.46
4:G:284:LEU:C	4:G:287:PRO:HD2	2.41	0.46
3:R:26:DA:H2''	3:R:27:DG:C8	2.50	0.46
4:A:189:ARG:NH2	4:A:591:GLN:HG3	2.31	0.46
4:G:155:ALA:HA	4:G:600:LEU:HD11	1.96	0.46
4:G:435:PHE:HZ	4:G:557:LEU:HD23	1.80	0.46
4:E:134:HIS:O	4:G:84:LYS:N	2.40	0.46
4:E:444:GLN:O	4:E:447:VAL:HG12	2.16	0.46
4:E:552:PRO:HG2	4:E:553:LYS:NZ	2.31	0.46
4:G:340:LEU:HA	4:G:343:ALA:HB3	1.98	0.46
4:A:162:ILE:HD12	4:A:607:PHE:HE2	1.80	0.46
4:A:276:ASN:HB3	4:A:416:ASN:ND2	2.29	0.46
4:C:322:THR:HA	4:C:325:MET:HG2	1.98	0.46
4:C:436:TYR:CD1	4:C:438:PRO:HD2	2.51	0.46
4:E:360:MET:HA	4:E:363:ILE:HG12	1.98	0.46
4:G:106:CYS:C	4:G:107:ARG:HD2	2.41	0.46
4:G:143:SER:O	4:G:146:THR:OG1	2.27	0.46
4:C:278:PHE:CZ	4:C:288:ILE:HG21	2.52	0.45
4:E:204:LEU:HD11	4:E:563:SER:HA	1.99	0.45
4:G:226:LYS:HA	4:G:229:LYS:NZ	2.32	0.45
4:G:284:LEU:HD23	4:G:409:LEU:HD22	1.96	0.45
4:A:293:ASN:HA	4:A:296:LYS:HE3	1.97	0.45
4:A:587:ASN:OD1	4:A:588:ARG:N	2.48	0.45
4:C:38:GLN:HG2	4:C:44:LEU:HD23	1.97	0.45
4:C:322:THR:HA	4:C:325:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:458:MET:HB3	4:E:557:LEU:HD21	1.99	0.45
4:G:397:SER:O	4:G:410:LYS:NZ	2.41	0.45
4:E:221:ALA:HB1	4:E:256:SER:HB3	1.99	0.45
4:G:290:ALA:O	4:G:294:ILE:HG12	2.16	0.45
4:K:26:GLY:HA3	4:K:31:TRP:CE3	2.51	0.45
4:A:67:ASN:OD1	4:A:68:LEU:HD12	2.16	0.45
4:A:370:ILE:O	4:A:374:LEU:HB2	2.17	0.45
4:G:316:PRO:HB2	4:G:318:ARG:HG3	1.98	0.45
4:K:5:ASP:O	4:K:9:VAL:HG23	2.16	0.45
4:A:286:MET:HB3	4:A:287:PRO:HD3	1.99	0.45
4:A:212:LYS:HZ3	4:A:213:SER:H	1.63	0.45
4:C:396:CYS:HB3	4:C:410:LYS:HB3	1.98	0.45
4:G:198:TYR:O	4:G:205:ARG:N	2.49	0.45
4:G:447:VAL:HA	4:G:450:ILE:HG12	1.98	0.45
4:A:322:THR:HA	4:A:325:MET:HG3	1.99	0.45
4:G:269:LEU:O	4:G:273:VAL:HG23	2.17	0.45
4:A:291:CYS:O	4:A:295:VAL:HG13	2.17	0.45
4:A:327:ARG:HH12	4:A:361:VAL:HG22	1.81	0.45
4:E:341:SER:HA	4:E:346:THR:HG22	1.99	0.45
4:G:414:ILE:HA	4:G:417:VAL:HG12	1.99	0.45
4:A:76:SER:HA	4:A:81:ARG:HH12	1.81	0.45
4:C:223:ASN:O	4:C:227:LYS:HG2	2.17	0.45
4:G:437:PRO:HG3	4:G:543:TRP:CE3	2.52	0.45
4:G:542:GLU:HA	4:G:545:ASN:HD22	1.81	0.45
4:A:396:CYS:HA	4:A:410:LYS:HE3	1.99	0.44
4:G:245:PHE:CE2	4:G:257:LEU:HD13	2.52	0.44
4:A:306:ARG:HG2	4:A:306:ARG:HH11	1.83	0.44
4:A:458:MET:HE1	4:A:553:LYS:HD3	1.99	0.44
4:C:435:PHE:CE2	4:C:561:LEU:HD23	2.52	0.44
2:N:4:DG:H2'	2:N:5:DA:C8	2.52	0.44
4:A:12:LYS:HG2	4:A:17:LEU:HD12	2.00	0.44
4:A:386:VAL:O	4:A:390:LEU:HG	2.17	0.44
4:A:415:LYS:O	4:A:419:ILE:HB	2.18	0.44
4:A:593:THR:O	4:A:597:LEU:HD23	2.18	0.44
4:C:167:LYS:O	4:C:170:VAL:HG12	2.17	0.44
4:E:333:TRP:HE3	4:E:354:LYS:HZ2	1.66	0.44
4:G:264:ASN:ND2	4:G:424:ASN:HB3	2.32	0.44
4:C:376:THR:HG22	4:C:379:SER:H	1.82	0.44
2:N:31:DA:OP1	4:E:59:LYS:NZ	2.44	0.44
4:A:75:ALA:HA	4:A:78:LYS:HG2	1.98	0.44
4:E:175:ALA:HB1	4:E:243:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:216:PHE:O	4:C:218:ARG:NH1	2.50	0.44
4:C:326:LEU:HA	4:C:329:ILE:HG12	1.98	0.44
4:E:118:ILE:HG22	4:E:122:LYS:NZ	2.31	0.44
4:A:292:LYS:HA	4:A:295:VAL:HG22	1.99	0.44
4:C:314:GLU:HG3	4:C:315:CYS:H	1.81	0.44
4:E:150:LYS:HZ1	4:G:96:GLU:N	2.16	0.44
4:E:162:ILE:O	4:E:165:GLU:HG2	2.18	0.44
4:E:245:PHE:CD2	4:E:257:LEU:HD22	2.53	0.44
4:G:353:ASN:OD1	4:G:354:LYS:N	2.50	0.44
4:C:214:LEU:HD23	4:C:227:LYS:HG3	1.99	0.44
4:E:23:ARG:HD3	4:E:24:HIS:N	2.32	0.44
4:G:254:VAL:HG22	4:G:262:ARG:HD3	2.00	0.44
4:C:298:PHE:HZ	4:C:336:VAL:HG23	1.83	0.44
4:C:364:LEU:HA	4:C:367:PHE:HB2	2.00	0.44
4:E:212:LYS:HB2	4:E:231:ILE:HD11	1.99	0.44
3:O:12:DT:H2''	3:O:13:DA:C8	2.53	0.43
2:Q:15:DA:N7	4:G:66:SER:OG	2.40	0.43
4:C:330:LEU:HD22	4:C:361:VAL:HG21	1.99	0.43
4:G:387:PRO:HD3	4:G:433:PHE:CE1	2.52	0.43
4:G:387:PRO:HD3	4:G:433:PHE:HE1	1.83	0.43
2:N:35:DA:H61	3:O:12:DT:H3	1.66	0.43
3:R:21:DA:H2''	3:R:22:DA:H5''	2.00	0.43
4:C:307:LEU:HD21	4:C:332:ASN:CG	2.44	0.43
4:G:47:GLY:HA2	4:G:60:TYR:O	2.17	0.43
4:E:392:VAL:HA	4:E:395:ILE:HG12	2.00	0.43
4:C:357:ILE:O	4:C:361:VAL:HG23	2.18	0.43
4:G:274:LEU:HD21	4:G:367:PHE:CE2	2.53	0.43
4:A:36:ASP:OD1	4:A:37:ILE:N	2.49	0.43
4:A:369:ARG:HH11	4:A:391:LYS:NZ	2.16	0.43
4:A:547:ASN:HB3	4:A:551:TYR:HD2	1.83	0.43
3:O:8:DC:C2'	3:O:9:DG:H5'	2.49	0.43
4:A:5:ASP:HA	4:A:8:GLU:OE1	2.18	0.43
4:A:37:ILE:HD11	4:A:50:PHE:HB3	2.01	0.43
4:A:346:THR:HA	4:A:349:ILE:HG12	2.01	0.43
4:A:437:PRO:HG3	4:A:543:TRP:CE3	2.54	0.43
4:C:520:PRO:O	4:C:523:GLU:HG2	2.19	0.43
4:E:386:VAL:N	4:E:387:PRO:HD2	2.34	0.43
4:A:13:ILE:HD13	4:A:18:TYR:HB2	2.01	0.43
4:A:327:ARG:HA	4:A:327:ARG:CZ	2.49	0.43
4:A:436:TYR:CE2	4:A:438:PRO:HD2	2.54	0.43
4:C:385:VAL:O	4:C:389:ILE:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:435:PHE:HE2	4:C:561:LEU:HD23	1.83	0.43
4:E:125:ILE:HG13	4:G:128:GLY:HA3	2.01	0.43
4:C:98:CYS:O	4:C:102:VAL:HG23	2.19	0.43
4:E:323:TYR:OH	4:E:365:ASP:OD1	2.29	0.43
4:G:524:PHE:O	4:G:528:ARG:HG3	2.19	0.43
4:A:327:ARG:HG2	4:A:327:ARG:HH11	1.84	0.43
4:C:64:GLN:HG2	4:C:66:SER:H	1.83	0.43
4:C:154:ASP:O	4:C:158:LYS:HG2	2.19	0.43
4:C:517:PRO:HB2	4:C:518:VAL:H	1.59	0.43
4:E:360:MET:SD	4:E:363:ILE:HD11	2.59	0.43
3:O:11:DA:H1'	3:O:12:DT:H5'	2.00	0.42
4:A:199:HIS:HA	4:A:204:LEU:HD13	2.00	0.42
4:E:418:ARG:NH1	4:E:422:GLU:OE2	2.52	0.42
2:Q:7:DC:OP1	4:E:589:ILE:HD12	2.19	0.42
4:C:214:LEU:HA	4:C:227:LYS:NZ	2.34	0.42
4:E:385:VAL:HG13	4:E:386:VAL:N	2.35	0.42
4:G:197:HIS:CG	4:G:565:PRO:HG3	2.54	0.42
2:N:3:DA:H2''	2:N:4:DG:C8	2.54	0.42
4:G:156:LYS:HE2	4:G:156:LYS:HB2	1.90	0.42
3:O:52:DA:H2''	3:O:53:DC:H5'	2.02	0.42
4:A:97:LYS:HD2	4:A:97:LYS:HA	1.82	0.42
4:A:170:VAL:HG23	4:A:175:ALA:HB2	2.02	0.42
4:A:247:THR:OG1	4:A:248:ASP:N	2.52	0.42
3:R:21:DA:H1'	3:R:22:DA:O4'	2.19	0.42
4:C:118:ILE:HA	4:C:121:ILE:HG12	2.02	0.42
4:C:437:PRO:HG2	4:C:538:PHE:HE2	1.84	0.42
4:E:176:SER:HB3	4:E:564:ILE:HD13	2.01	0.42
3:O:2:DA:H2''	3:O:3:DA:C8	2.54	0.42
3:O:54:DG:N7	3:O:55:DC:N4	2.68	0.42
4:E:6:ASN:HD21	4:E:48:TRP:CG	2.37	0.42
4:G:386:VAL:HA	4:G:389:ILE:HD12	2.00	0.42
4:G:436:TYR:CD1	4:G:437:PRO:HD2	2.53	0.42
1:M:2:DC:H2''	1:M:3:DG:C8	2.55	0.42
4:A:9:VAL:HA	4:A:12:LYS:HE2	2.01	0.42
4:C:213:SER:O	4:C:227:LYS:NZ	2.51	0.42
4:E:167:LYS:HA	4:E:170:VAL:HG12	2.00	0.42
4:G:12:LYS:O	4:G:16:GLY:N	2.52	0.42
2:N:19:DG:OP1	4:I:59:LYS:NZ	2.51	0.42
4:A:212:LYS:HA	4:A:212:LYS:HD2	1.84	0.42
4:E:606:ASN:C	4:E:606:ASN:HD22	2.26	0.42
4:G:270:LEU:HD23	4:G:371:PHE:CE1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:407:ALA:O	4:G:411:VAL:HG23	2.20	0.42
4:A:155:ALA:O	4:A:159:LYS:HB2	2.20	0.42
4:E:103:VAL:HG23	4:G:597:LEU:HD13	2.01	0.42
4:E:327:ARG:HD3	4:E:361:VAL:HG13	2.02	0.42
2:Q:4:DG:H1'	4:E:585:LYS:HE2	2.02	0.42
4:A:142:PRO:HG3	4:C:95:ILE:HD13	2.02	0.42
4:A:252:ASN:OD1	4:A:253:VAL:N	2.52	0.42
4:A:442:MET:HE3	4:A:444:GLN:HB2	2.02	0.42
4:C:199:HIS:CE1	4:C:204:LEU:HG	2.55	0.42
4:E:374:LEU:HD12	4:E:374:LEU:HA	1.90	0.42
4:G:15:GLN:HG3	4:G:17:LEU:HD23	2.01	0.41
4:A:225:TYR:O	4:A:228:LEU:HG	2.20	0.41
4:C:527:TYR:HA	4:C:530:GLU:OE1	2.20	0.41
4:E:248:ASP:HB2	4:E:265:CYS:HB3	2.02	0.41
4:G:570:ALA:O	4:G:574:THR:HG23	2.19	0.41
2:N:1:DA:H2''	2:N:2:DG:H8	1.85	0.41
3:O:53:DC:H5''	4:A:251:ALA:HB1	2.02	0.41
4:E:48:TRP:CD1	4:E:59:LYS:HA	2.55	0.41
4:E:245:PHE:HD2	4:E:257:LEU:HD13	1.85	0.41
3:R:50:DT:H6	3:R:50:DT:H2'	1.62	0.41
4:C:285:ASN:O	4:C:288:ILE:HG22	2.20	0.41
4:C:286:MET:HB3	4:C:287:PRO:HD3	2.03	0.41
4:G:19:LYS:HG3	4:G:38:GLN:HE21	1.86	0.41
3:O:5:DT:H6	3:O:5:DT:H2'	1.70	0.41
4:A:284:LEU:C	4:A:287:PRO:HD2	2.45	0.41
4:C:437:PRO:HG2	4:C:538:PHE:CE2	2.55	0.41
4:E:140:LEU:HD12	4:G:91:LYS:HD2	2.01	0.41
4:E:252:ASN:OD1	4:E:253:VAL:N	2.52	0.41
3:O:46:DT:H72	3:O:47:DG:C6	2.55	0.41
4:A:133:GLU:HG3	4:C:129:ALA:HB3	2.02	0.41
4:A:273:VAL:HG11	4:A:417:VAL:HG12	2.02	0.41
4:C:25:LYS:HD2	4:C:25:LYS:HA	1.91	0.41
4:C:148:SER:O	4:C:151:VAL:HG12	2.20	0.41
4:E:411:VAL:HA	4:E:414:ILE:HG22	2.01	0.41
2:N:7:DC:H2''	2:N:8:DA:H8	1.86	0.41
1:P:4:DT:H6	1:P:4:DT:H2'	1.76	0.41
4:A:388:SER:O	4:A:392:VAL:HG23	2.20	0.41
4:E:25:LYS:HA	4:E:25:LYS:HD3	1.76	0.41
4:E:82:GLU:HG2	4:E:83:LEU:O	2.20	0.41
4:E:544:TRP:HE3	4:E:555:SER:HA	1.85	0.41
4:G:369:ARG:O	4:G:372:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:581:ILE:O	4:G:586:ARG:NH2	2.44	0.41
4:A:212:LYS:NZ	4:A:213:SER:H	2.19	0.41
4:A:227:LYS:O	4:A:231:ILE:HG12	2.20	0.41
4:A:369:ARG:O	4:A:372:LYS:N	2.53	0.41
4:C:578:ALA:O	4:C:582:ILE:HG22	2.21	0.41
4:I:32:ASN:OD1	4:I:33:VAL:N	2.54	0.41
4:E:215:ASP:C	4:E:216:PHE:HD2	2.29	0.41
4:E:283:GLU:HA	4:E:286:MET:HE1	2.02	0.41
4:A:122:LYS:HB2	4:A:122:LYS:HE3	1.84	0.41
4:A:213:SER:O	4:A:227:LYS:NZ	2.51	0.41
4:A:405:ASP:HA	4:A:408:LYS:HE3	2.02	0.41
4:C:93:GLU:OE2	4:C:93:GLU:HA	2.20	0.41
4:G:268:HIS:HD2	4:G:319:TRP:CH2	2.38	0.41
4:G:425:LEU:HD12	4:G:425:LEU:HA	1.95	0.41
4:G:435:PHE:HD2	4:G:544:TRP:CZ2	2.39	0.41
4:K:39:LYS:HB2	4:K:43:THR:HB	2.02	0.41
4:A:95:ILE:HG13	4:C:150:LYS:HE3	2.03	0.41
4:A:225:TYR:O	4:A:229:LYS:HG3	2.21	0.41
4:C:414:ILE:HA	4:C:417:VAL:HG12	2.03	0.41
4:C:440:LEU:HD23	4:C:440:LEU:HA	1.93	0.41
4:E:85:THR:HG22	4:E:86:VAL:N	2.35	0.41
4:G:175:ALA:H	4:G:244:LYS:NZ	2.18	0.41
4:G:405:ASP:OD1	4:G:406:ILE:N	2.52	0.41
4:A:189:ARG:NH1	4:A:591:GLN:HE21	2.19	0.40
1:M:4:DT:H6	1:M:4:DT:H2'	1.74	0.40
4:C:282:PRO:HA	4:C:285:ASN:HB2	2.03	0.40
4:E:154:ASP:O	4:E:157:GLU:HG3	2.21	0.40
4:E:525:GLU:HB3	4:E:529:LYS:NZ	2.36	0.40
4:G:200:GLU:HG3	4:G:205:ARG:HE	1.86	0.40
4:A:559:LEU:HD23	4:A:562:LEU:HD21	2.03	0.40
2:N:1:DA:H5''	4:A:372:LYS:HA	2.04	0.40
1:P:6:DA:H3'	4:G:249:ARG:NH2	2.36	0.40
4:A:327:ARG:NH1	4:A:361:VAL:HG13	2.35	0.40
4:A:369:ARG:HA	4:A:372:LYS:HG2	2.02	0.40
4:C:403:VAL:HG12	4:C:406:ILE:HG13	2.02	0.40
4:E:92:LYS:HD2	4:E:92:LYS:HA	1.84	0.40
3:O:29:DC:OP1	4:A:59:LYS:HG2	2.21	0.40
4:A:436:TYR:CD2	4:A:438:PRO:HD2	2.56	0.40
4:E:120:MET:HE1	4:G:117:PHE:HZ	1.87	0.40
4:E:124:PHE:HA	4:E:127:VAL:HG12	2.03	0.40
4:G:33:VAL:HG22	4:G:77:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:185:ASN:OD1	4:G:186:TYR:N	2.55	0.40
4:G:427:ILE:O	4:G:431:THR:HG23	2.21	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	
4	A	546/612 (89%)	516 (94%)	30 (6%)	0	100	100
4	C	546/612 (89%)	527 (96%)	19 (4%)	0	100	100
4	E	546/612 (89%)	514 (94%)	32 (6%)	0	100	100
4	G	546/612 (89%)	519 (95%)	27 (5%)	0	100	100
4	I	72/612 (12%)	70 (97%)	2 (3%)	0	100	100
4	K	72/612 (12%)	71 (99%)	1 (1%)	0	100	100
All	All	2328/3672 (63%)	2217 (95%)	111 (5%)	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 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	
4	A	504/565 (89%)	504 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	504/565 (89%)	504 (100%)	0	100	100
4	E	504/565 (89%)	503 (100%)	1 (0%)	87	85
4	G	504/565 (89%)	504 (100%)	0	100	100
4	I	68/565 (12%)	68 (100%)	0	100	100
4	K	68/565 (12%)	68 (100%)	0	100	100
All	All	2152/3390 (64%)	2151 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	580	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	38	GLN
4	A	79	GLN
4	A	260	ASN
4	A	302	ASN
4	A	351	HIS
4	A	416	ASN
4	C	79	GLN
4	C	199	HIS
4	C	260	ASN
4	C	353	ASN
4	C	362	ASN
4	E	6	ASN
4	E	64	GLN
4	E	100	GLN
4	E	272	ASN
4	E	285	ASN
4	E	304	GLN
4	E	320	ASN
4	E	416	ASN
4	E	545	ASN
4	E	606	ASN
4	G	259	ASN
4	G	358	GLN
4	G	416	ASN

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Mol	Chain	Res	Type
4	G	606	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 Map visualisation

This section contains visualisations of the EMDB entry EMD-28034. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.