



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:36 pm GMT

PDB ID : 1FIU
Title : TETRAMERIC RESTRICTION ENDONUCLEASE NGOMIV IN COMPLEX WITH CLEAVED DNA
Authors : Deibert, M.; Grazulis, S.; Sasnauskas, G.; Siksnys, V.; Huber, R.
Deposited on : 2000-08-07
Resolution : 1.60 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

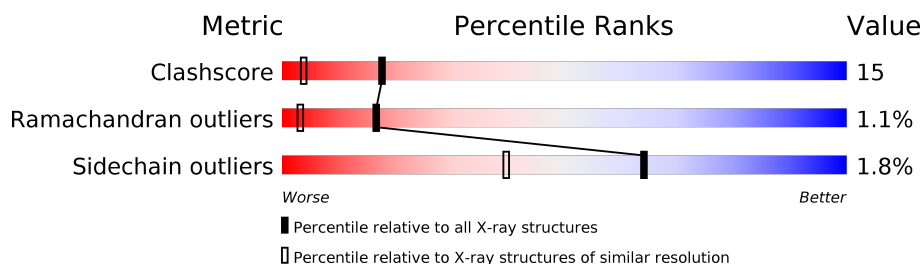
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)






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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	4	<div><div></div><div>50%50%</div></div>
1	F	4	<div><div></div><div>25%25%50%</div></div>
1	G	4	<div><div></div><div>100%</div></div>
1	H	4	<div><div></div><div>50%50%</div></div>
2	I	7	<div><div></div><div>57%29%14%</div></div>
2	J	7	<div><div></div><div>57%29%14%</div></div>
2	K	7	<div><div></div><div>57%43%</div></div>

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Mol	Chain	Length	Quality of chain
2	L	7	 71% 29%
3	A	286	 79% 18% •
3	B	286	 79% 19% •
3	C	286	 74% 22% •
3	D	286	 77% 21% •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11147 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*TP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	4	Total	C	N	O	P	0	0	0
			80	39	15	23	3			
1	F	4	Total	C	N	O	P	0	0	0
			80	39	15	23	3			
1	G	4	Total	C	N	O	P	0	0	0
			80	39	15	23	3			
1	H	4	Total	C	N	O	P	0	0	0
			80	39	15	23	3			

- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*CP*GP*GP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	7	Total	C	N	O	P	0	0	0
			143	66	27	43	7			
2	J	7	Total	C	N	O	P	0	0	0
			143	66	27	43	7			
2	K	7	Total	C	N	O	P	0	0	0
			143	66	27	43	7			
2	L	7	Total	C	N	O	P	0	0	0
			143	66	27	43	7			

- Molecule 3 is a protein called TYPE II RESTRICTION ENZYME NGOMI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	286	Total	C	N	O	S	0	0	0
			2238	1399	404	429	6			
3	B	286	Total	C	N	O	S	0	0	0
			2238	1399	404	429	6			
3	C	286	Total	C	N	O	S	0	0	0
			2238	1399	404	429	6			
3	D	286	Total	C	N	O	S	0	0	0
			2238	1399	404	429	6			

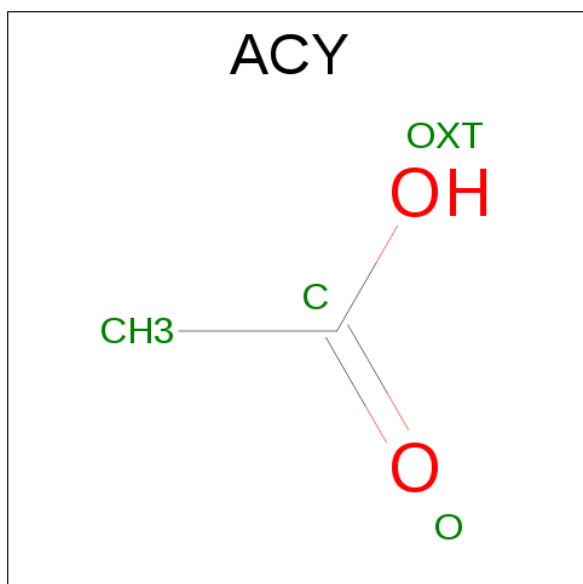
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLN	ASN	CONFLICT	UNP P31032
B	2	GLN	ASN	CONFLICT	UNP P31032
C	2	GLN	ASN	CONFLICT	UNP P31032
D	2	GLN	ASN	CONFLICT	UNP P31032

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	K	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	15	Total O 15 15	0	0
6	I	36	Total O 36 36	0	0
6	F	12	Total O 12 12	0	0
6	J	35	Total O 35 35	0	0
6	G	14	Total O 14 14	0	0
6	K	32	Total O 32 32	0	0
6	H	17	Total O 17 17	0	0
6	L	32	Total O 32 32	0	0
6	A	258	Total O 258 258	0	0
6	B	273	Total O 273 273	0	0
6	C	252	Total O 252 252	0	0
6	D	303	Total O 303 303	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

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

Chain E: 



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

Chain F: 



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

Chain G: 

There are no outlier residues recorded for this chain.

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

Chain H: 



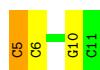
- Molecule 2: DNA (5'-D(P*CP*CP*GP*GP*CP*GP*C)-3')

Chain I: 



- Molecule 2: DNA (5'-D(P*CP*CP*GP*GP*CP*GP*C)-3')

Chain J: 



- Molecule 2: DNA (5'-D(P*CP*CP*GP*GP*CP*GP*C)-3')

Chain K: 57% 43%



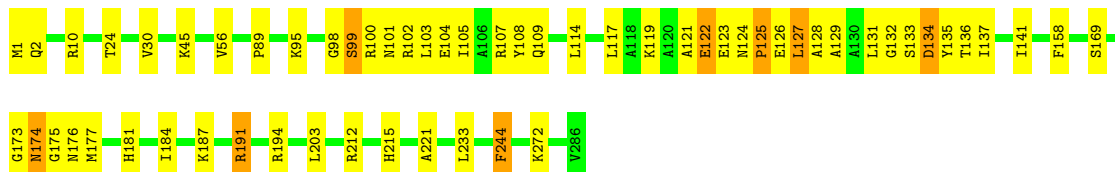
- Molecule 2: DNA (5'-D(P*CP*CP*GP*GP*CP*GP*C)-3')

Chain L: 71% 29%



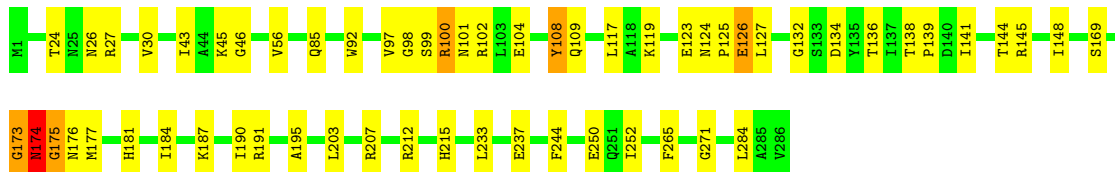
- Molecule 3: TYPE II RESTRICTION ENZYME NGOMI

Chain A: 79% 18%



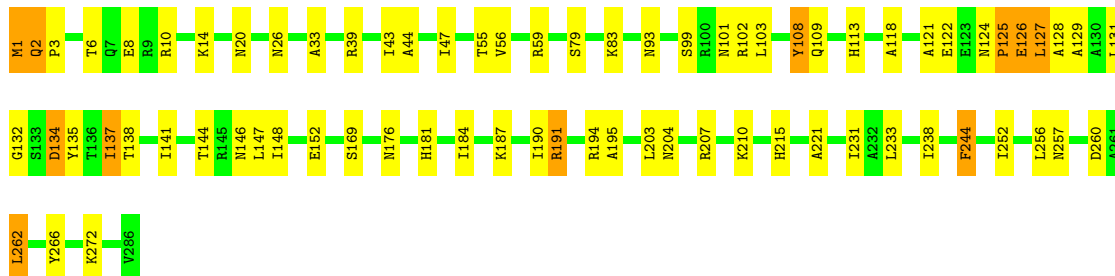
- Molecule 3: TYPE II RESTRICTION ENZYME NGOMI

Chain B: 79% 19%



- Molecule 3: TYPE II RESTRICTION ENZYME NGOMI

Chain C: 74% 22%

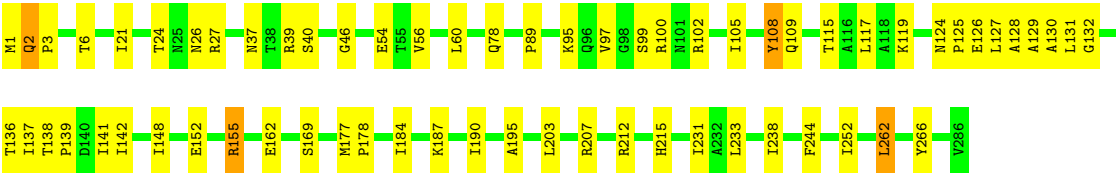


- Molecule 3: TYPE II RESTRICTION ENZYME NGOMI

Chain D:

77%

21%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.40Å 91.13Å 149.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.26 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (17.26-1.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.173 , 0.204	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11147	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	E	0.49	0/89	0.79	0/136
1	F	0.64	0/89	0.87	0/136
1	G	0.56	0/89	0.96	0/136
1	H	0.65	0/89	0.82	0/136
2	I	0.96	1/159 (0.6%)	0.92	0/241
2	J	1.08	1/159 (0.6%)	0.88	0/241
2	K	1.02	1/159 (0.6%)	1.01	1/241 (0.4%)
2	L	0.96	1/159 (0.6%)	0.96	0/241
3	A	0.52	0/2275	0.75	1/3083 (0.0%)
3	B	0.48	0/2275	0.71	1/3083 (0.0%)
3	C	0.53	0/2275	0.75	2/3083 (0.1%)
3	D	0.54	0/2275	0.73	0/3083
All	All	0.56	4/10092 (0.0%)	0.76	5/13840 (0.0%)

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	E	0	2
1	F	0	2
1	H	0	3
2	I	0	1
2	J	0	1
2	K	0	1
2	L	0	1
3	A	0	1
3	B	0	1
3	C	0	1
3	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	5	DC	OP3-P	-8.06	1.51	1.61
2	I	5	DC	OP3-P	-7.72	1.51	1.61
2	L	5	DC	OP3-P	-6.87	1.52	1.61
2	K	5	DC	OP3-P	-6.32	1.53	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	59	ARG	NE-CZ-NH2	-5.28	117.66	120.30
3	A	191	ARG	N-CA-C	-5.24	96.86	111.00
3	B	191	ARG	N-CA-C	-5.10	97.23	111.00
3	C	191	ARG	N-CA-C	-5.07	97.31	111.00
2	K	6	DC	OP2-P-O3'	5.06	116.32	105.20

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	108	TYR	Sidechain
3	B	108	TYR	Sidechain
3	C	108	TYR	Sidechain
3	D	108	TYR	Sidechain
1	E	2	DG	Sidechain
1	E	4	DG	Sidechain
1	F	2	DG	Sidechain
1	F	4	DG	Sidechain
1	H	2	DG	Sidechain
1	H	3	DC	Sidechain
1	H	4	DG	Sidechain
2	I	10	DG	Sidechain
2	J	10	DG	Sidechain
2	K	10	DG	Sidechain
2	L	10	DG	Sidechain

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	E	80	0	47	2	0
1	F	80	0	47	2	0
1	G	80	0	47	0	0
1	H	80	0	47	5	0
2	I	143	0	78	1	0
2	J	143	0	78	1	0
2	K	143	0	78	0	0
2	L	143	0	78	0	0
3	A	2238	0	2234	72	0
3	B	2238	0	2234	71	0
3	C	2238	0	2234	93	0
3	D	2238	0	2234	70	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
5	D	4	0	3	0	0
6	A	258	0	0	14	0
6	B	273	0	0	12	0
6	C	252	0	0	22	0
6	D	303	0	0	17	0
6	E	15	0	0	1	0
6	F	12	0	0	0	0
6	G	14	0	0	0	0
6	H	17	0	0	2	0
6	I	36	0	0	0	0
6	J	35	0	0	0	0
6	K	32	0	0	0	0
6	L	32	0	0	0	0
All	All	11147	0	9448	296	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 15.

All (296) 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)
3:B:46:GLY:HA3	3:B:252:ILE:HD12	1.19	1.14
3:D:124:ASN:HD22	3:D:127:LEU:HG	0.97	1.09
3:D:124:ASN:ND2	3:D:127:LEU:HG	1.69	1.06
3:D:231:ILE:HD11	3:D:238:ILE:HD11	1.41	1.02
3:B:109:GLN:NE2	3:B:176:ASN:HD21	1.59	1.00
3:C:126:GLU:O	3:C:128:ALA:N	1.95	0.98
3:B:43:ILE:HA	3:B:252:ILE:HD13	1.54	0.90
3:A:127:LEU:HD22	3:A:131:LEU:HD11	1.51	0.90
3:B:46:GLY:CA	3:B:252:ILE:HD12	2.04	0.88
3:C:126:GLU:HG3	3:C:127:LEU:N	1.90	0.86
3:C:231:ILE:HD11	3:C:238:ILE:HD11	1.55	0.86
3:C:126:GLU:HG3	3:C:127:LEU:H	1.41	0.86
3:C:47:ILE:HG13	3:C:252:ILE:HD13	1.58	0.85
3:B:109:GLN:NE2	3:B:176:ASN:ND2	2.26	0.83
3:C:134:ASP:OD2	3:C:204:ASN:ND2	2.11	0.83
3:B:174:ASN:C	3:B:176:ASN:H	1.82	0.82
3:D:78:GLN:HG3	6:D:1102:HOH:O	1.80	0.82
3:C:129:ALA:O	6:C:8027:HOH:O	1.97	0.81
3:A:101:ASN:HB3	3:A:104:GLU:HB2	1.62	0.81
3:C:14:LYS:HE2	6:C:7963:HOH:O	1.79	0.81
3:C:203:LEU:HD21	3:C:207:ARG:NH2	1.95	0.81
3:B:109:GLN:HE22	3:B:176:ASN:HD21	1.27	0.81
3:B:97:VAL:HG11	3:B:138:THR:HG21	1.63	0.80
3:C:124:ASN:OD1	3:C:125:PRO:HD2	1.81	0.80
3:C:101:ASN:HB3	3:C:138:THR:HG21	1.64	0.80
3:D:124:ASN:HD22	3:D:127:LEU:CG	1.87	0.79
3:A:124:ASN:HB3	3:A:127:LEU:HD12	1.65	0.79
3:C:126:GLU:O	3:C:129:ALA:N	2.15	0.79
3:A:132:GLY:HA2	3:B:233:LEU:HB3	1.63	0.79
3:C:118:ALA:O	3:C:122:GLU:HG2	1.83	0.79
3:B:119:LYS:HD2	6:B:3560:HOH:O	1.81	0.78
3:C:43:ILE:HG23	3:C:252:ILE:HD11	1.63	0.78
3:C:135:TYR:O	3:C:137:ILE:HG13	1.83	0.78
3:B:203:LEU:HD21	3:B:207:ARG:CZ	2.13	0.78
3:B:85:GLN:OE1	6:B:3476:HOH:O	2.03	0.77
6:A:5813:HOH:O	3:B:126:GLU:HA	1.84	0.76
3:B:145:ARG:NH2	6:B:3543:HOH:O	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:ASP:CG	3:C:204:ASN:HD21	1.89	0.76
3:C:135:TYR:C	3:C:137:ILE:H	1.89	0.75
3:A:119:LYS:O	3:A:122:GLU:HG2	1.86	0.75
3:C:43:ILE:HG23	3:C:252:ILE:CD1	2.17	0.75
3:B:98:GLY:HA3	3:B:100:ARG:CD	2.17	0.74
3:D:162:GLU:CD	3:D:162:GLU:H	1.92	0.73
3:B:98:GLY:C	3:B:100:ARG:N	2.39	0.73
3:D:203:LEU:HD21	3:D:207:ARG:CZ	2.19	0.73
3:C:55:THR:HB	6:C:7825:HOH:O	1.88	0.72
3:B:98:GLY:C	3:B:100:ARG:H	1.90	0.72
3:B:43:ILE:HA	3:B:252:ILE:CD1	2.19	0.72
3:A:126:GLU:N	6:A:5732:HOH:O	2.23	0.71
3:A:133:SER:O	3:A:136:THR:HB	1.90	0.71
3:D:231:ILE:HD11	3:D:238:ILE:CD1	2.18	0.71
3:B:174:ASN:C	3:B:176:ASN:N	2.44	0.71
6:A:5776:HOH:O	3:D:1:MET:SD	2.48	0.70
3:C:101:ASN:CB	3:C:138:THR:HG21	2.20	0.70
3:B:46:GLY:HA3	3:B:252:ILE:CD1	2.12	0.70
3:B:125:PRO:O	3:B:126:GLU:HB3	1.92	0.69
3:C:134:ASP:HB3	6:D:1242:HOH:O	1.92	0.69
3:D:100:ARG:HG3	6:D:1263:HOH:O	1.92	0.69
3:D:203:LEU:HD21	3:D:207:ARG:NH2	2.06	0.69
3:C:101:ASN:HB2	3:C:138:THR:OG1	1.94	0.68
3:B:125:PRO:O	3:B:126:GLU:CB	2.42	0.68
1:H:2:DG:H3'	6:C:8021:HOH:O	1.93	0.68
3:C:93:ASN:HD21	3:C:146:ASN:HD21	1.41	0.67
3:D:26:ASN:OD1	3:D:27:ARG:HD3	1.94	0.67
3:D:97:VAL:HG11	3:D:138:THR:HG21	1.76	0.66
3:C:124:ASN:CG	3:C:125:PRO:HD2	2.14	0.66
3:C:203:LEU:HD21	3:C:207:ARG:CZ	2.25	0.66
3:A:173:GLY:C	3:A:175:GLY:H	1.98	0.66
3:B:237:GLU:HG3	6:B:3429:HOH:O	1.95	0.66
3:C:39:ARG:HH12	3:C:260:ASP:CG	1.98	0.66
3:D:1:MET:HB2	3:D:6:THR:HG21	1.78	0.66
3:B:127:LEU:HD22	3:D:117:LEU:HD23	1.77	0.65
3:B:85:GLN:HE22	3:B:92:TRP:HD1	1.42	0.65
3:C:121:ALA:O	3:C:124:ASN:O	2.14	0.64
3:A:134:ASP:C	3:A:136:THR:N	2.51	0.64
3:A:2:GLN:HE22	3:A:10:ARG:NH1	1.96	0.64
3:A:124:ASN:OD1	6:A:5732:HOH:O	2.15	0.64
3:D:2:GLN:H	3:D:2:GLN:CD	2.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:187:LYS:NZ	6:D:1299:HOH:O	2.25	0.64
3:B:109:GLN:NE2	3:B:176:ASN:OD1	2.31	0.63
3:B:174:ASN:O	3:B:176:ASN:N	2.31	0.63
3:B:97:VAL:O	6:B:3556:HOH:O	2.15	0.63
3:C:127:LEU:HB2	6:C:8022:HOH:O	1.98	0.63
3:C:47:ILE:HG13	3:C:252:ILE:CD1	2.27	0.63
3:C:126:GLU:CG	3:C:127:LEU:N	2.62	0.63
3:A:2:GLN:NE2	3:A:10:ARG:NH1	2.47	0.62
3:A:121:ALA:C	3:A:123:GLU:H	2.03	0.62
3:D:100:ARG:N	6:D:1263:HOH:O	2.33	0.62
3:A:2:GLN:HE22	3:A:10:ARG:HH12	1.45	0.62
3:D:102:ARG:HG2	3:D:136:THR:O	1.99	0.62
3:B:187:LYS:NZ	6:B:3605:HOH:O	2.26	0.62
3:D:105:ILE:HG12	6:D:1298:HOH:O	2.01	0.61
3:D:119:LYS:HE2	6:D:1288:HOH:O	2.01	0.61
3:A:134:ASP:C	3:A:136:THR:H	2.04	0.61
3:A:181:HIS:HD2	6:D:1013:HOH:O	1.82	0.61
3:B:98:GLY:HA3	3:B:100:ARG:HG3	1.82	0.61
3:D:102:ARG:HH21	3:D:137:ILE:CG1	2.14	0.61
3:C:93:ASN:HD21	3:C:146:ASN:ND2	1.98	0.61
3:C:14:LYS:HG3	6:C:7984:HOH:O	2.00	0.60
3:C:207:ARG:HD2	6:C:7945:HOH:O	2.01	0.60
3:B:173:GLY:O	3:B:175:GLY:N	2.33	0.60
3:D:231:ILE:CD1	3:D:238:ILE:CD1	2.79	0.60
3:B:203:LEU:HD21	3:B:207:ARG:NH2	2.16	0.59
3:C:26:ASN:ND2	6:C:7915:HOH:O	2.33	0.59
3:B:98:GLY:HA3	3:B:100:ARG:NE	2.17	0.59
3:C:215:HIS:HD2	6:C:7865:HOH:O	1.85	0.59
3:D:231:ILE:CD1	3:D:238:ILE:HD11	2.24	0.58
3:C:2:GLN:H	3:C:3:PRO:HD2	1.69	0.58
3:A:135:TYR:O	3:A:137:ILE:HG13	2.03	0.58
3:A:173:GLY:HA2	6:A:5798:HOH:O	2.04	0.58
3:C:124:ASN:HB3	6:C:8023:HOH:O	2.04	0.57
3:D:109:GLN:HE22	3:D:169:SER:HA	1.68	0.57
3:B:97:VAL:HG11	3:B:138:THR:CG2	2.32	0.57
3:B:101:ASN:OD1	3:B:104:GLU:HB2	2.04	0.57
3:D:177:MET:HB3	3:D:178:PRO:HD2	1.86	0.57
6:B:3503:HOH:O	3:C:272:LYS:HE2	2.05	0.56
3:D:215:HIS:HD2	6:D:1076:HOH:O	1.87	0.56
6:B:3378:HOH:O	3:C:181:HIS:HD2	1.88	0.56
3:A:109:GLN:HE22	3:A:169:SER:CB	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:215:HIS:HD2	6:A:5566:HOH:O	1.89	0.56
3:B:215:HIS:HD2	6:B:3341:HOH:O	1.87	0.56
1:E:4:DG:H4'	3:B:99:SER:HB2	1.88	0.56
3:C:134:ASP:CB	6:D:1242:HOH:O	2.51	0.56
3:B:98:GLY:HA3	3:B:100:ARG:CG	2.36	0.56
3:C:256:LEU:O	3:C:257:ASN:HB3	2.06	0.56
3:A:158:PHE:CZ	3:D:3:PRO:HG3	2.41	0.56
3:D:99:SER:N	6:D:1263:HOH:O	2.39	0.56
3:A:125:PRO:HG2	6:A:5732:HOH:O	2.06	0.55
3:D:100:ARG:NE	6:D:1104:HOH:O	2.38	0.55
3:D:115:THR:O	3:D:119:LYS:HG2	2.06	0.55
3:A:105:ILE:HD13	3:A:137:ILE:HB	1.87	0.55
3:A:2:GLN:NE2	3:A:10:ARG:HH12	2.02	0.55
3:A:117:LEU:HD23	3:C:127:LEU:CD2	2.36	0.55
3:C:1:MET:HG3	3:C:6:THR:HG22	1.88	0.55
3:D:155:ARG:HD3	6:D:1186:HOH:O	2.06	0.55
3:B:181:HIS:HD2	6:C:7867:HOH:O	1.89	0.54
3:C:231:ILE:CD1	3:C:238:ILE:HD11	2.31	0.54
3:D:126:GLU:O	3:D:129:ALA:N	2.40	0.54
3:B:124:ASN:HB2	3:B:127:LEU:HD12	1.90	0.54
3:D:109:GLN:HE22	3:D:169:SER:CA	2.21	0.54
3:C:134:ASP:CG	3:C:204:ASN:ND2	2.59	0.54
3:D:109:GLN:HE22	3:D:169:SER:CB	2.21	0.54
3:A:187:LYS:NZ	6:A:5799:HOH:O	2.29	0.54
3:B:109:GLN:NE2	3:B:176:ASN:CG	2.61	0.53
3:C:132:GLY:HA2	3:D:233:LEU:HB3	1.90	0.53
3:A:124:ASN:ND2	3:A:127:LEU:HG	2.24	0.53
3:D:2:GLN:CD	3:D:2:GLN:N	2.61	0.53
3:C:127:LEU:HG	6:C:8023:HOH:O	2.07	0.53
3:D:125:PRO:O	3:D:128:ALA:HB3	2.09	0.53
3:C:108:TYR:CE2	3:C:144:THR:HG21	2.45	0.52
3:B:30:VAL:HG21	3:B:45:LYS:HA	1.91	0.52
3:D:97:VAL:CG1	3:D:138:THR:HG21	2.39	0.52
3:B:123:GLU:C	3:B:125:PRO:HD3	2.29	0.52
3:C:231:ILE:HD11	3:C:238:ILE:CD1	2.34	0.52
3:C:187:LYS:NZ	6:C:8017:HOH:O	2.37	0.51
3:C:257:ASN:HB3	6:C:8029:HOH:O	2.09	0.51
3:D:124:ASN:HB3	3:D:127:LEU:HD12	1.92	0.51
3:C:233:LEU:HB3	3:D:132:GLY:HA2	1.93	0.51
3:A:127:LEU:HD22	3:A:131:LEU:CD1	2.34	0.51
3:A:127:LEU:O	3:A:131:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:176:ASN:ND2	6:A:5790:HOH:O	2.44	0.51
3:C:20:ASN:ND2	3:C:55:THR:HG21	2.25	0.51
3:B:190:ILE:HG23	3:B:195:ALA:HB2	1.93	0.51
3:C:1:MET:CE	3:C:10:ARG:HB2	2.41	0.51
3:C:231:ILE:HG13	3:C:238:ILE:HD13	1.93	0.51
3:B:26:ASN:OD1	3:B:27:ARG:HD3	2.10	0.51
3:C:126:GLU:O	3:C:127:LEU:C	2.48	0.50
3:B:43:ILE:CA	3:B:252:ILE:HD13	2.36	0.50
3:A:212:ARG:HD2	3:D:215:HIS:CE1	2.46	0.50
3:C:231:ILE:CD1	3:C:238:ILE:CD1	2.89	0.50
3:A:173:GLY:C	3:A:175:GLY:N	2.65	0.50
3:C:14:LYS:HE3	6:C:7984:HOH:O	2.10	0.50
3:D:141:ILE:HB	3:D:184:ILE:HB	1.93	0.49
3:C:127:LEU:O	3:C:131:LEU:HG	2.12	0.49
3:A:176:ASN:OD1	3:A:177:MET:N	2.46	0.49
3:C:101:ASN:CB	3:C:138:THR:CG2	2.89	0.49
3:D:125:PRO:HG2	3:D:126:GLU:H	1.78	0.49
3:B:102:ARG:HG3	6:B:3433:HOH:O	2.13	0.49
3:B:117:LEU:HD23	3:D:127:LEU:CD2	2.42	0.49
3:D:126:GLU:O	3:D:127:LEU:C	2.51	0.49
3:A:203:LEU:HD23	6:A:5800:HOH:O	2.11	0.49
3:B:169:SER:O	3:B:176:ASN:ND2	2.45	0.49
3:C:147:LEU:CD1	3:C:176:ASN:HB3	2.43	0.49
3:A:133:SER:O	3:A:136:THR:CB	2.60	0.49
3:B:181:HIS:HE1	3:B:284:LEU:O	1.96	0.48
3:B:176:ASN:OD1	3:B:177:MET:N	2.46	0.48
3:C:203:LEU:CD2	3:C:207:ARG:CZ	2.91	0.48
3:D:262:LEU:HD22	3:D:266:TYR:CE1	2.48	0.48
3:A:109:GLN:OE1	3:A:176:ASN:OD1	2.32	0.48
3:C:125:PRO:C	6:C:8022:HOH:O	2.51	0.48
3:A:173:GLY:O	3:A:175:GLY:N	2.47	0.48
3:C:138:THR:O	6:C:7780:HOH:O	2.20	0.48
3:A:121:ALA:C	3:A:123:GLU:N	2.68	0.48
3:A:129:ALA:CB	3:B:271:GLY:HA3	2.44	0.48
1:E:2:DG:H8	6:E:440:HOH:O	1.97	0.48
3:A:215:HIS:CE1	3:D:212:ARG:HD2	2.49	0.47
3:A:126:GLU:OE2	3:C:210:LYS:NZ	2.39	0.47
3:A:272:LYS:NZ	6:A:5663:HOH:O	2.47	0.47
3:D:215:HIS:HE1	6:D:1087:HOH:O	1.97	0.47
3:A:134:ASP:O	3:A:136:THR:N	2.47	0.47
3:A:174:ASN:N	6:A:5762:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:5:DC:H2'	2:J:6:DC:C6	2.50	0.47
3:C:135:TYR:C	3:C:137:ILE:N	2.62	0.47
3:D:102:ARG:HH21	3:D:137:ILE:HG12	1.79	0.47
3:B:117:LEU:HD23	3:D:127:LEU:HD23	1.97	0.47
3:D:108:TYR:CD2	3:D:178:PRO:HG2	2.50	0.47
3:C:126:GLU:CB	6:C:8026:HOH:O	2.63	0.47
3:D:2:GLN:OE1	3:D:2:GLN:N	2.46	0.47
3:A:109:GLN:OE1	3:A:176:ASN:ND2	2.46	0.47
3:B:98:GLY:CA	3:B:100:ARG:HG3	2.44	0.47
3:A:203:LEU:CD2	6:A:5800:HOH:O	2.63	0.47
3:A:215:HIS:HE1	6:A:5565:HOH:O	1.98	0.46
3:B:250:GLU:HG3	3:B:265:PHE:CE2	2.51	0.46
3:D:127:LEU:O	3:D:131:LEU:HG	2.15	0.46
3:A:124:ASN:CB	3:A:127:LEU:HD12	2.41	0.46
3:A:191:ARG:HB2	3:A:194:ARG:HG2	1.98	0.46
3:D:39:ARG:NE	6:D:1301:HOH:O	2.44	0.46
3:A:124:ASN:CG	3:A:127:LEU:HB2	2.37	0.46
3:D:54:GLU:HB2	6:D:1251:HOH:O	2.16	0.46
3:C:56:VAL:HG11	6:C:7915:HOH:O	2.16	0.46
3:D:109:GLN:NE2	3:D:169:SER:CB	2.79	0.45
3:C:33:ALA:HB2	3:C:44:ALA:CB	2.46	0.45
1:H:3:DC:H5''	6:H:1223:HOH:O	2.17	0.45
3:C:8:GLU:OE2	3:C:79:SER:OG	2.29	0.45
3:A:141:ILE:HB	3:A:184:ILE:HB	1.98	0.45
1:F:1:DT:H2''	1:F:2:DG:C8	2.52	0.45
3:A:121:ALA:O	3:A:123:GLU:N	2.50	0.45
3:A:233:LEU:HB3	3:B:132:GLY:HA2	1.99	0.45
3:C:191:ARG:HB2	3:C:194:ARG:HG2	1.99	0.45
3:D:138:THR:HA	3:D:139:PRO:HD3	1.85	0.45
3:A:89:PRO:HD2	3:D:89:PRO:HD2	1.99	0.45
3:D:95:LYS:HE2	3:D:142:ILE:HD11	1.99	0.45
3:D:155:ARG:HH11	3:D:155:ARG:HG2	1.81	0.45
3:D:126:GLU:OE2	3:D:130:ALA:HB2	2.17	0.45
3:B:138:THR:HA	3:B:139:PRO:HD3	1.80	0.44
3:C:262:LEU:HD22	3:C:266:TYR:CE1	2.52	0.44
3:A:221:ALA:HA	3:A:244:PHE:CD2	2.51	0.44
3:A:30:VAL:HG21	3:A:45:LYS:HA	1.98	0.44
3:C:190:ILE:HG23	3:C:195:ALA:HB2	1.99	0.44
3:A:126:GLU:CD	3:C:113:HIS:HB3	2.37	0.44
3:C:135:TYR:O	3:C:137:ILE:N	2.49	0.44
3:C:231:ILE:HG13	3:C:238:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:190:ILE:HG23	3:D:195:ALA:HB2	1.99	0.44
3:A:124:ASN:OD1	3:A:124:ASN:C	2.56	0.44
3:A:124:ASN:HA	3:A:125:PRO:HD2	1.47	0.44
3:B:124:ASN:O	3:B:125:PRO:C	2.56	0.44
3:B:102:ARG:NH2	6:B:3411:HOH:O	2.50	0.43
3:D:24:THR:O	3:D:56:VAL:HA	2.18	0.43
3:C:215:HIS:HE1	6:C:7827:HOH:O	2.00	0.43
3:B:215:HIS:HE1	6:B:3342:HOH:O	2.00	0.43
3:D:109:GLN:NE2	3:D:169:SER:HB3	2.33	0.43
3:C:148:ILE:CG2	3:C:152:GLU:HB3	2.48	0.43
3:B:108:TYR:CE2	3:B:144:THR:HG21	2.53	0.43
3:C:221:ALA:HA	3:C:244:PHE:CD2	2.54	0.43
3:A:126:GLU:HG3	3:C:210:LYS:NZ	2.34	0.43
3:A:124:ASN:O	3:A:127:LEU:HB2	2.18	0.43
3:B:141:ILE:HB	3:B:184:ILE:HB	2.01	0.42
3:A:126:GLU:HG2	3:C:113:HIS:HB2	2.01	0.42
3:C:55:THR:HB	6:C:7909:HOH:O	2.18	0.42
3:A:109:GLN:HE22	3:A:169:SER:CA	2.32	0.42
1:F:4:DG:H4'	3:A:99:SER:HB3	2.01	0.42
3:B:100:ARG:HG3	3:B:100:ARG:H	1.37	0.42
3:C:83:LYS:NZ	6:C:7831:HOH:O	2.51	0.42
2:I:5:DC:H2'	2:I:6:DC:C6	2.55	0.42
3:D:21:ILE:HD13	3:D:60:LEU:CD1	2.48	0.42
3:B:134:ASP:C	3:B:136:THR:N	2.72	0.42
3:A:24:THR:O	3:A:56:VAL:HA	2.19	0.42
1:H:2:DG:H2''	1:H:3:DC:OP2	2.19	0.42
3:A:102:ARG:O	3:A:103:LEU:HB2	2.19	0.42
3:B:145:ARG:NH2	3:B:148:ILE:HD11	2.34	0.42
3:C:141:ILE:HB	3:C:184:ILE:HB	2.00	0.42
3:C:43:ILE:HG23	3:C:252:ILE:HD12	2.00	0.42
3:C:127:LEU:HA	3:C:127:LEU:HD23	1.80	0.42
1:H:1:DT:C2'	1:H:2:DG:C8	3.03	0.42
1:H:3:DC:H1'	6:H:947:HOH:O	2.20	0.42
3:B:109:GLN:O	3:C:272:LYS:NZ	2.53	0.41
3:C:126:GLU:C	3:C:128:ALA:N	2.71	0.41
3:A:95:LYS:NZ	3:A:107:ARG:NH2	2.69	0.41
3:B:212:ARG:HD2	3:C:215:HIS:CE1	2.55	0.41
3:A:122:GLU:HG3	3:A:123:GLU:HG3	2.02	0.41
3:D:46:GLY:HA3	3:D:252:ILE:HG12	2.01	0.41
3:C:102:ARG:O	3:C:103:LEU:HB2	2.20	0.41
3:C:43:ILE:CG2	3:C:252:ILE:HD11	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:24:THR:O	3:B:56:VAL:HA	2.21	0.41
3:B:98:GLY:HA3	3:B:100:ARG:HD2	1.99	0.41
3:C:109:GLN:OE1	3:C:169:SER:HB3	2.20	0.41
3:D:148:ILE:CG2	3:D:152:GLU:HB3	2.51	0.41
3:D:37:ASN:HB3	3:D:40:SER:HB3	2.01	0.41
3:A:114:LEU:HD23	3:A:117:LEU:HD12	2.03	0.41
3:B:98:GLY:O	3:B:100:ARG:N	2.53	0.41
3:A:109:GLN:HE22	3:A:169:SER:HA	1.86	0.40
3:A:98:GLY:O	3:A:100:ARG:N	2.54	0.40
3:C:108:TYR:CZ	3:C:144:THR:HG21	2.57	0.40
3:A:125:PRO:O	3:A:128:ALA:N	2.54	0.40
3:B:101:ASN:CG	3:B:104:GLU:HB2	2.42	0.40
3:D:119:LYS:HG2	6:D:1288:HOH:O	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 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	
3	A	284/286 (99%)	273 (96%)	7 (2%)	4 (1%)	13	2
3	B	284/286 (99%)	273 (96%)	7 (2%)	4 (1%)	13	2
3	C	284/286 (99%)	271 (95%)	9 (3%)	4 (1%)	13	2
3	D	284/286 (99%)	273 (96%)	11 (4%)	0	100	100
All	All	1136/1144 (99%)	1090 (96%)	34 (3%)	12 (1%)	17	3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	125	PRO
3	B	126	GLU

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Mol	Chain	Res	Type
3	B	174	ASN
3	C	125	PRO
3	C	127	LEU
3	C	137	ILE
3	A	99	SER
3	A	122	GLU
3	A	174	ASN
3	B	175	GLY
3	B	173	GLY
3	C	2	GLN

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	
3	A	241/241 (100%)	237 (98%)	4 (2%)	66	42
3	B	241/241 (100%)	238 (99%)	3 (1%)	75	58
3	C	241/241 (100%)	235 (98%)	6 (2%)	53	25
3	D	241/241 (100%)	237 (98%)	4 (2%)	66	42
All	All	964/964 (100%)	947 (98%)	17 (2%)	64	40

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1	MET
3	A	127	LEU
3	A	134	ASP
3	A	244	PHE
3	B	100	ARG
3	B	174	ASN
3	B	244	PHE
3	C	1	MET
3	C	99	SER
3	C	126	GLU
3	C	134	ASP

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Mol	Chain	Res	Type
3	C	244	PHE
3	C	262	LEU
3	D	2	GLN
3	D	155	ARG
3	D	244	PHE
3	D	262	LEU

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

Mol	Chain	Res	Type
3	A	2	GLN
3	A	20	ASN
3	A	67	ASN
3	A	93	ASN
3	A	146	ASN
3	A	156	ASN
3	A	181	HIS
3	A	215	HIS
3	B	20	ASN
3	B	85	GLN
3	B	93	ASN
3	B	109	GLN
3	B	146	ASN
3	B	174	ASN
3	B	181	HIS
3	B	215	HIS
3	C	20	ASN
3	C	26	ASN
3	C	146	ASN
3	C	181	HIS
3	C	215	HIS
3	D	20	ASN
3	D	109	GLN
3	D	124	ASN
3	D	215	HIS

5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ACY	A	2001	4	1,3,3	2.88	1 (100%)	0,3,3	0.00	-
5	ACY	B	3002	4	1,3,3	1.14	0	0,3,3	0.00	-
5	ACY	C	4003	4	1,3,3	2.10	1 (100%)	0,3,3	0.00	-
5	ACY	D	5004	4	1,3,3	3.14	1 (100%)	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ACY	A	2001	4	-	0/0/0/0	0/0/0/0
5	ACY	B	3002	4	-	0/0/0/0	0/0/0/0
5	ACY	C	4003	4	-	0/0/0/0	0/0/0/0
5	ACY	D	5004	4	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	4003	ACY	CH3-C	2.10	1.51	1.48
5	A	2001	ACY	CH3-C	2.88	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	5004	ACY	CH3-C	3.14	1.52	1.48

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.