



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:25 AM UTC

PDB ID : 1FIU / pdb_00001fiu
Title : TETRAMERIC RESTRICTION ENDONUCLEASE NGOMIV IN COMPLEX WITH CLEAVED DNA
Authors : Deibert, M.; Grazulis, S.; Sasnauskas, G.; Siksnyis, 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

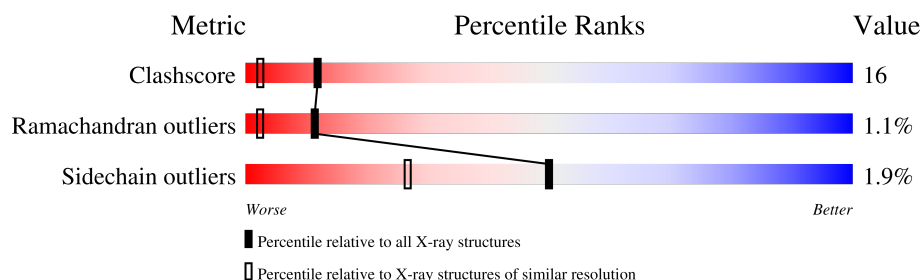
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	4	
1	F	4	
1	G	4	
1	H	4	
2	I	7	
2	J	7	
2	K	7	
2	L	7	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	A	286	 77% 17% 5%
3	B	286	 77% 19% •
3	C	286	 72% 23% 5%
3	D	286	 74% 24% •

2 Entry composition

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			

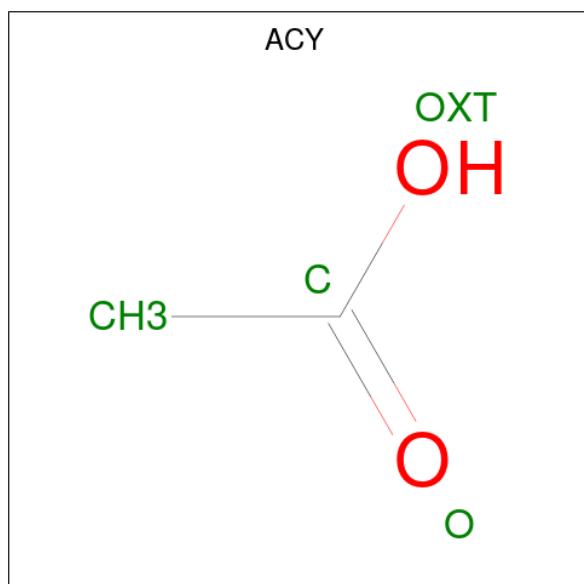
There are 4 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is ACETIC ACID (CCD ID: 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, 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.

Note EDS was not executed.

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

Chain E: 

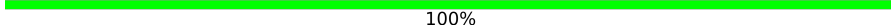


- Molecule 1: DNA (5'-D(*TP*GP*CP*G)-3')

Chain F: 



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

Chain G: 

There are no outlier residues recorded for this chain.

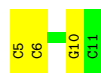
- Molecule 1: DNA (5'-D(*TP*GP*CP*G)-3')

Chain H: 



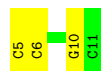
- Molecule 2: DNA (5'-D(P*CP*CP*GP*GP*CP*GP*C)-3')

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:  86% 14%



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

Chain L:  86% 14%



- Molecule 3: TYPE II RESTRICTION ENZYME NGOMI

Chain A:  77% 17% 5%



- Molecule 3: TYPE II RESTRICTION ENZYME NGOMI

Chain B:  77% 19% 4%



- Molecule 3: TYPE II RESTRICTION ENZYME NGOMI

Chain C:  72% 23% 5%



- Molecule 3: TYPE II RESTRICTION ENZYME NGOMI

Chain D:  74% 24% 2%



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: MG, ACY

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	0.33	0/89	0.78	0/136
1	F	0.45	0/89	0.91	0/136
1	G	0.34	0/89	0.99	0/136
1	H	0.39	0/89	0.94	0/136
2	I	0.45	0/159	0.90	0/241
2	J	0.51	0/159	0.85	0/241
2	K	0.55	0/159	0.96	0/241
2	L	0.48	0/159	0.91	0/241
3	A	0.60	0/2275	1.08	16/3083 (0.5%)
3	B	0.57	0/2275	1.02	11/3083 (0.4%)
3	C	0.63	0/2275	1.04	11/3083 (0.4%)
3	D	0.65	1/2275 (0.0%)	1.00	10/3083 (0.3%)
All	All	0.60	1/10092 (0.0%)	1.02	48/13840 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
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

Continued on next page...

Continued from previous page...

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	197	ASN	CG-OD1	5.13	1.33	1.23

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	99	SER	N-CA-C	-10.68	100.05	112.87
3	A	127	LEU	N-CA-C	-10.10	99.27	111.69
3	A	175	GLY	N-CA-C	-10.00	101.33	115.43
3	B	104	GLU	N-CA-C	-8.77	101.63	111.71
3	A	124	ASN	CA-C-N	8.43	130.38	119.84
3	A	124	ASN	C-N-CA	8.43	130.38	119.84
3	A	97	VAL	N-CA-C	7.52	117.58	110.74
3	A	191	ARG	N-CA-C	-7.41	96.86	109.24
3	A	173	GLY	N-CA-C	7.30	123.38	114.69
3	C	124	ASN	CA-C-N	7.24	128.89	119.84
3	C	124	ASN	C-N-CA	7.24	128.89	119.84
3	B	191	ARG	N-CA-C	-7.19	97.23	109.24
3	A	109	GLN	N-CA-C	7.16	119.70	111.11
3	C	191	ARG	N-CA-C	-7.14	97.31	109.24
3	C	104	GLU	N-CA-C	-7.06	103.59	111.71
3	B	259	GLU	N-CA-C	7.03	118.59	111.07
3	A	224	THR	N-CA-C	7.03	118.50	109.72
3	A	31	SER	N-CA-C	6.84	121.08	112.87
3	C	256	LEU	N-CA-C	6.55	121.11	113.18
3	B	224	THR	N-CA-C	6.38	117.69	109.72
3	B	31	SER	N-CA-C	6.23	120.35	112.87
3	D	259	GLU	N-CA-C	6.20	118.04	111.28
3	D	21	ILE	N-CA-C	-6.19	104.71	110.53
3	D	191	ARG	N-CA-C	-6.18	98.92	109.24
3	A	259	GLU	N-CA-C	6.12	118.45	111.11
3	A	21	ILE	N-CA-C	-5.98	104.91	110.53
3	C	125	PRO	N-CA-C	5.96	124.74	112.47
3	C	99	SER	N-CA-C	5.95	118.53	111.33
3	C	31	SER	N-CA-C	5.78	119.80	112.87
3	C	224	THR	N-CA-C	5.76	116.92	109.72
3	B	109	GLN	N-CA-C	5.75	118.01	111.11
3	B	138	THR	CA-C-N	5.75	126.07	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	138	THR	C-N-CA	5.75	126.07	119.92
3	B	21	ILE	N-CA-C	-5.74	105.14	110.53
3	D	31	SER	N-CA-C	5.66	119.80	113.01
3	A	207	ARG	N-CA-C	5.56	118.11	111.71
3	C	96	GLN	N-CA-C	-5.54	100.77	109.25
3	A	176	ASN	N-CA-C	5.53	118.30	110.50
3	D	148	ILE	N-CA-C	5.50	116.50	108.53
3	D	224	THR	N-CA-C	5.46	116.55	109.72
3	A	101	ASN	N-CA-C	5.42	117.98	108.56
3	A	95	LYS	N-CA-C	5.26	117.25	108.99
3	D	173	GLY	N-CA-C	5.14	125.37	113.18
3	D	2	GLN	CA-C-N	-5.12	114.50	119.78
3	D	2	GLN	C-N-CA	-5.12	114.50	119.78
3	D	34	ASP	N-CA-C	-5.06	98.34	107.75
3	B	125	PRO	N-CA-C	-5.04	103.19	111.15
3	C	143	VAL	N-CA-C	-5.01	101.09	108.11

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	73	0
3	B	2238	0	2234	74	0
3	C	2238	0	2234	95	0
3	D	2238	0	2234	76	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	13	0
6	B	273	0	0	13	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	306	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 16.

All (306) 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:B:174:ASN:C	3:B:176:ASN:H	1.82	0.86
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: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:C:134:ASP:CG	3:C:204:ASN:HD21	1.89	0.80
3:C:135:TYR:C	3:C:137:ILE:H	1.89	0.80
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:D:162:GLU:CD	3:D:162:GLU:H	1.92	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
3:A:119:LYS:O	3:A:122:GLU:HG2	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:98:GLY:C	3:B:100:ARG:H	1.90	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:B:174:ASN:C	3:B:176:ASN:N	2.44	0.74
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:43:ILE:HA	3:B:252:ILE:CD1	2.19	0.72
3:B:98:GLY:C	3:B:100:ARG:N	2.39	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:C:124:ASN:CG	3:C:125:PRO:HD2	2.14	0.71
6:A:5776:HOH:O	3:D:1:MET:SD	2.48	0.70
3:A:173:GLY:C	3:A:175:GLY:H	1.98	0.70
3:C:39:ARG:HH12	3:C:260:ASP:CG	1.98	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:D:2:GLN:CD	3:D:2:GLN:H	2.01	0.68
1:H:2:DG:H3'	6:C:8021:HOH:O	1.93	0.68
3:B:125:PRO:O	3:B:126:GLU:CB	2.42	0.68
3:A:121:ALA:C	3:A:123:GLU:H	2.03	0.67
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:203:LEU:HD21	3:C:207:ARG:CZ	2.25	0.66
3:A:134:ASP:C	3:A:136:THR:H	2.04	0.66
3:B:237:GLU:HG3	6:B:3429:HOH:O	1.95	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: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:A:134:ASP:C	3:A:136:THR:N	2.51	0.64
3:B:109:GLN:NE2	3:B:176:ASN:OD1	2.31	0.63
3:B:97:VAL:O	6:B:3556:HOH:O	2.15	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:174:ASN:O	3:B:176:ASN:N	2.31	0.63
3:C:127:LEU:HB2	6:C:8022:HOH:O	1.98	0.63
3:A:163:ASN:HB2	3:D:1:MET:HE1	1.81	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: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: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: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:85:GLN:HE22	3:B:92:TRP:CD1	2.20	0.59
3:B:98:GLY:HA3	3:B:100:ARG:NE	2.17	0.59
3:C:134:ASP:CG	3:C:204:ASN:ND2	2.59	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:D:2:GLN:CD	3:D:2:GLN:N	2.61	0.58
3:C:187:LYS:NZ	6:C:8017:HOH:O	2.37	0.58
3:B:109:GLN:NE2	3:B:176:ASN:CG	2.61	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:A:163:ASN:CB	3:D:1:MET:HE1	2.35	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:B:123:GLU:C	3:B:125:PRO:HD3	2.29	0.56
6:B:3378:HOH:O	3:C:181:HIS:HD2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:126:GLU:O	3:C:127:LEU:C	2.48	0.56
3:D:215:HIS:HD2	6:D:1076:HOH:O	1.87	0.56
3:A:109:GLN:HE22	3:A:169:SER:CB	2.19	0.56
3:A:215:HIS:HD2	6:A:5566:HOH:O	1.89	0.56
1:E:4:DG:H4'	3:B:99:SER:HB2	1.88	0.56
3:B:215:HIS:HD2	6:B:3341:HOH:O	1.87	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:A:158:PHE:CZ	3:D:3:PRO:HG3	2.41	0.56
3:C:256:LEU:O	3:C:257:ASN:HB3	2.06	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:125:PRO:C	6:C:8022:HOH:O	2.51	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:D:109:GLN:HE22	3:D:169:SER:CB	2.21	0.54
3:D:126:GLU:O	3:D:127:LEU:C	2.51	0.54
3:D:112:ALA:HB1	3:D:177:MET:HE1	1.90	0.54
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: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:A:121:ALA:C	3:A:123:GLU:N	2.68	0.52
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:C:231:ILE:HD11	3:C:238:ILE:CD1	2.34	0.52
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:127:LEU:O	3:A:131:LEU:HG	2.10	0.51
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:A:124:ASN:CG	3:A:127:LEU:HB2	2.37	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:D:112:ALA:CB	3:D:177:MET:HE1	2.41	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:A:126:GLU:CD	3:C:113:HIS:HB3	2.37	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:A:124:ASN:OD1	3:A:124:ASN:C	2.56	0.48
3:B:181:HIS:HE1	3:B:284:LEU:O	1.96	0.48
3:B:124:ASN:O	3:B:125:PRO:C	2.56	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: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
1:E:2:DG:H8	6:E:440:HOH:O	1.97	0.48
3:A:129:ALA:CB	3:B:271:GLY:HA3	2.44	0.48
3:B:134:ASP:C	3:B:136:THR:N	2.72	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: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

Continued on next page...

Continued from previous page...

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:A:174:ASN:N	6:A:5762:HOH:O	2.47	0.47
3:B:117:LEU:HD23	3:D:127:LEU:HD23	1.97	0.47
3:C:126:GLU:CB	6:C:8026:HOH:O	2.63	0.47
3:D:2:GLN:N	3:D:2:GLN:OE1	2.46	0.47
3:D:102:ARG:HH21	3:D:137:ILE:HG12	1.79	0.47
3:D:108:TYR:CD2	3:D:178:PRO:HG2	2.50	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:C:126:GLU:C	3:C:128:ALA:N	2.71	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: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:B:188:TRP:NE1	6:B:3606:HOH:O	2.48	0.45
1:H:3:DC:H5''	6:H:1223:HOH:O	2.17	0.45
3:C:33:ALA:HB2	3:C:44:ALA:CB	2.46	0.45
3:C:8:GLU:OE2	3:C:79:SER:OG	2.29	0.45
1:F:1:DT:H2''	1:F:2:DG:C8	2.52	0.45
3:A:141:ILE:HB	3:A:184:ILE:HB	1.98	0.45
3:A:121:ALA:O	3:A:123:GLU:N	2.50	0.45
3:A:89:PRO:HD2	3:D:89:PRO:HD2	1.99	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:B:101:ASN:CG	3:B:104:GLU:HB2	2.42	0.45
3:D:95:LYS:HE2	3:D:142:ILE:HD11	1.99	0.45
3:C:173:GLY:O	3:C:174:ASN:C	2.59	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:30:VAL:HG21	3:A:45:LYS:HA	1.98	0.44
3:A:221:ALA:HA	3:A:244:PHE:CD2	2.51	0.44
3:C:190:ILE:HG23	3:C:195:ALA:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:134:ASP:C	3:B:136:THR:H	2.23	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
3:D:190:ILE:HG23	3:D:195:ALA:HB2	1.99	0.44
3:D:126:GLU:C	3:D:126:GLU:CD	2.83	0.44
3:C:135:TYR:C	3:C:137:ILE:N	2.62	0.44
3:A:124:ASN:HA	3:A:125:PRO:HD2	1.47	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:A:126:GLU:HG2	3:C:113:HIS:HB2	2.01	0.42
3:B:141:ILE:HB	3:B:184:ILE:HB	2.01	0.42
3:C:55:THR:HB	6:C:7909:HOH:O	2.18	0.42
1:F:4:DG:H4'	3:A:99:SER:HB3	2.01	0.42
3:A:109:GLN:HE22	3:A:169:SER:CA	2.32	0.42
3:B:100:ARG:H	3:B:100:ARG:HG3	1.37	0.42
2:I:5:DC:H2'	2:I:6:DC:C6	2.55	0.42
3:C:83:LYS:NZ	6:C:7831:HOH:O	2.51	0.42
3:D:21:ILE:HD13	3:D:60:LEU:CD1	2.48	0.42
1:H:2:DG:H2''	1:H:3:DC:OP2	2.19	0.42
3:A:24:THR:O	3:A:56:VAL:HA	2.19	0.42
3:A:125:PRO:C	3:A:127:LEU:H	2.28	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:43:ILE:HG23	3:C:252:ILE:HD12	2.00	0.42
3:C:141:ILE:HB	3:C:184:ILE:HB	2.00	0.42
3:B:187:LYS:NZ	6:B:3605:HOH:O	2.26	0.42
3:D:174:ASN:C	3:D:176:ASN:H	2.28	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:C:127:LEU:HD23	3:C:127:LEU:HA	1.80	0.42
3:B:109:GLN:O	3:C:272:LYS:NZ	2.53	0.41
3:D:187:LYS:NZ	6:D:1299:HOH:O	2.25	0.41
3:A:95:LYS:NZ	3:A:107:ARG:NH2	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:135:TYR:C	3:C:135:TYR:CD1	2.98	0.41
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:43:ILE:CG2	3:C:252:ILE:HD11	2.44	0.41
3:C:109:GLN:OE1	3:C:169:SER:HB3	2.20	0.41
3:D:37:ASN:HB3	3:D:40:SER:HB3	2.01	0.41
3:D:148:ILE:CG2	3:D:152:GLU:HB3	2.51	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:15:LYS:NZ	6:A:5678:HOH:O	2.53	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: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%)	9	1
3	B	284/286 (99%)	273 (96%)	7 (2%)	4 (1%)	9	1
3	C	284/286 (99%)	271 (95%)	9 (3%)	4 (1%)	9	1
3	D	284/286 (99%)	273 (96%)	11 (4%)	0	100	100
All	All	1136/1144 (99%)	1090 (96%)	34 (3%)	12 (1%)	11	2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	125	PRO
3	B	126	GLU
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%)	53	30
3	B	241/241 (100%)	236 (98%)	5 (2%)	47	23
3	C	241/241 (100%)	235 (98%)	6 (2%)	42	18
3	D	241/241 (100%)	238 (99%)	3 (1%)	63	43
All	All	964/964 (100%)	946 (98%)	18 (2%)	50	27

All (18) 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	137	ILE
3	B	100	ARG
3	B	105	ILE
3	B	174	ASN
3	B	244	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	250	GLU
3	C	1	MET
3	C	99	SER
3	C	109	GLN
3	C	126	GLU
3	C	134	ASP
3	C	262	LEU
3	D	2	GLN
3	D	244	PHE
3	D	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	2	GLN
3	A	20	ASN
3	A	96	GLN
3	A	181	HIS
3	A	215	HIS
3	B	20	ASN
3	B	67	ASN
3	B	85	GLN
3	B	93	ASN
3	B	109	GLN
3	B	124	ASN
3	B	146	ASN
3	B	174	ASN
3	B	181	HIS
3	B	215	HIS
3	B	254	GLN
3	C	20	ASN
3	C	26	ASN
3	C	146	ASN
3	C	181	HIS
3	C	215	HIS
3	C	257	ASN
3	D	20	ASN
3	D	109	GLN
3	D	124	ASN
3	D	176	ASN
3	D	215	HIS

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 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	3,3,3	1.66	1 (33%)	3,3,3	1.25	0
5	ACY	D	5004	4	3,3,3	0.95	0	3,3,3	1.70	1 (33%)
5	ACY	C	4003	4	3,3,3	1.57	1 (33%)	3,3,3	1.18	0
5	ACY	B	3002	4	3,3,3	0.90	0	3,3,3	1.81	1 (33%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	ACY	O-C	2.39	1.32	1.22
5	C	4003	ACY	O-C	2.29	1.32	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3002	ACY	O-C-CH3	-2.49	112.33	122.53
5	D	5004	ACY	O-C-CH3	-2.33	112.96	122.53

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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.