



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:05 PM UTC

PDB ID : 3CD2 / pdb_00003cd2
Title : LIGAND INDUCED CONFORMATIONAL CHANGES IN THE CRYSTAL STRUCTURES OF PNEUMOCYSTIS CARINII DIHYDROFOLATE REDUCTASE COMPLEXES WITH FOLATE AND NADP+
Authors : Cody, V.; Galitsky, N.; Rak, D.; Luft, J.; Pangborn, W.; Queener, S.
Deposited on : 1999-03-16
Resolution : 2.50 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

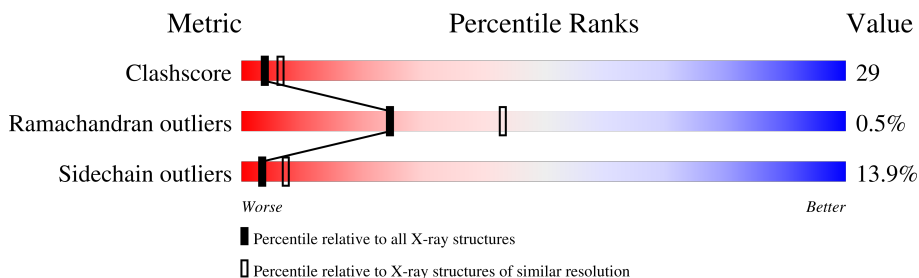
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	A	206	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1815 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

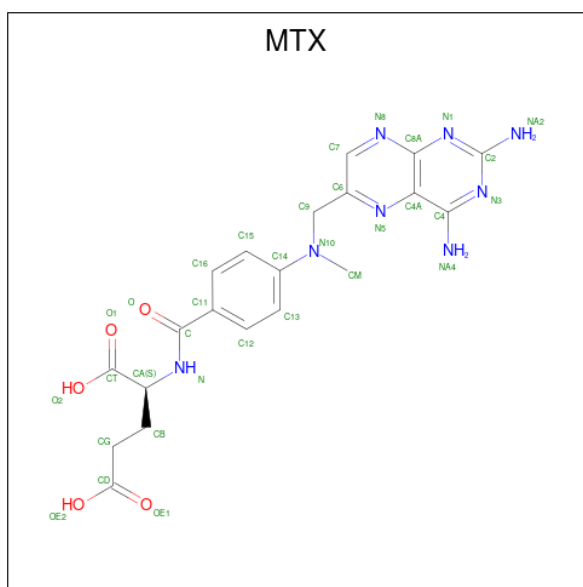
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	206	1686	1086	288	305	7	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is METHOTREXATE (CCD ID: MTX) (formula: C₂₀H₂₂N₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	33	20	8	5	0	0

- Molecule 4 is water.

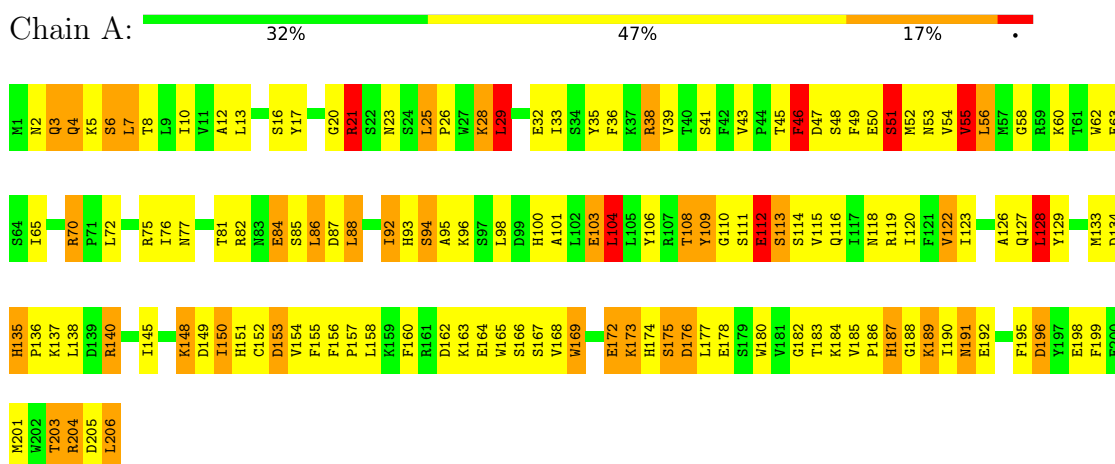
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		

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.

Note EDS was not executed.

- Molecule 1: DIHYDROFOLATE REDUCTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.42Å 43.56Å 61.66Å 90.00° 94.89° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	96.3 (8.00-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1815	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

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: MTX, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	6.68	1/1728 (0.1%)	2.73	136/2330 (5.8%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	PHE	C-O	274.40	4.69	1.24

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	PHE	O-C-N	-49.70	56.49	122.59
1	A	204	ARG	CD-NE-CZ	25.40	159.96	124.40
1	A	46	PHE	CA-C-O	19.65	148.61	120.51
1	A	55	VAL	CB-CA-C	16.03	131.83	110.99
1	A	119	ARG	NE-CZ-NH1	12.11	133.61	121.50
1	A	157	PRO	N-CA-C	10.54	127.00	114.03
1	A	77	ASN	CA-CB-CG	10.42	123.02	112.60
1	A	55	VAL	N-CA-CB	-10.30	98.92	111.90
1	A	51	SER	N-CA-C	10.24	125.67	110.52
1	A	103	GLU	CB-CG-CD	9.29	128.40	112.60
1	A	50	GLU	CA-CB-CG	9.29	132.68	114.10
1	A	134	ASP	CA-CB-CG	8.75	121.35	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	GLU	CB-CG-CD	8.72	127.43	112.60
1	A	205	ASP	CA-CB-CG	8.66	121.27	112.60
1	A	140	ARG	NE-CZ-NH2	8.66	126.99	119.20
1	A	196	ASP	CA-C-O	-8.65	110.80	120.32
1	A	103	GLU	CA-CB-CG	8.52	131.15	114.10
1	A	21	ARG	CD-NE-CZ	8.42	136.19	124.40
1	A	176	ASP	CA-CB-CG	-8.15	104.45	112.60
1	A	153	ASP	CA-C-N	8.13	133.79	123.14
1	A	153	ASP	C-N-CA	8.13	133.79	123.14
1	A	112	GLU	N-CA-C	-8.08	102.06	111.03
1	A	38	ARG	NE-CZ-NH1	8.04	129.54	121.50
1	A	10	ILE	CB-CA-C	7.88	121.83	110.33
1	A	122	VAL	CA-C-O	-7.63	112.36	120.53
1	A	167	SER	N-CA-C	-7.63	103.77	113.23
1	A	140	ARG	CD-NE-CZ	-7.58	113.78	124.40
1	A	21	ARG	CG-CD-NE	7.50	128.51	112.00
1	A	129	TYR	N-CA-C	-7.35	103.20	111.14
1	A	187	HIS	CA-C-O	-7.27	112.46	120.38
1	A	13	LEU	N-CA-CB	-7.26	99.06	111.69
1	A	168	VAL	CB-CA-C	7.21	120.31	111.80
1	A	87	ASP	N-CA-C	-7.09	101.17	110.53
1	A	158	LEU	CB-CA-C	7.03	121.94	109.65
1	A	92	ILE	N-CA-CB	7.02	120.51	111.67
1	A	151	HIS	CA-CB-CG	-6.87	106.93	113.80
1	A	29	LEU	N-CA-CB	-6.86	99.36	110.69
1	A	94	SER	CA-C-O	-6.82	113.14	121.06
1	A	8	THR	N-CA-CB	6.81	123.32	111.00
1	A	156	PHE	CB-CA-C	6.79	120.41	109.41
1	A	6	SER	CA-C-O	-6.62	113.41	121.36
1	A	122	VAL	N-CA-C	-6.60	98.24	107.80
1	A	50	GLU	CG-CD-OE1	6.58	133.54	118.40
1	A	199	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	41	SER	CA-C-O	6.50	126.76	119.41
1	A	35	TYR	N-CA-C	-6.46	104.23	111.28
1	A	72	LEU	CB-CA-C	6.45	119.44	110.16
1	A	119	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	A	153	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	51	SER	CA-C-O	6.34	129.21	121.72
1	A	128	LEU	N-CA-CB	-6.32	100.10	110.40
1	A	160	PHE	CA-CB-CG	6.28	120.08	113.80
1	A	38	ARG	CD-NE-CZ	6.23	133.12	124.40
1	A	198	GLU	CA-C-N	6.20	130.68	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	GLU	C-N-CA	6.20	130.68	122.30
1	A	87	ASP	N-CA-CB	6.19	119.21	110.36
1	A	36	PHE	CB-CA-C	6.14	120.69	110.92
1	A	16	SER	CA-C-N	6.14	132.69	123.05
1	A	16	SER	C-N-CA	6.14	132.69	123.05
1	A	12	ALA	CA-C-O	-6.12	113.76	120.24
1	A	151	HIS	CB-CA-C	6.07	119.73	109.84
1	A	112	GLU	CA-CB-CG	6.06	126.22	114.10
1	A	192	GLU	CG-CD-OE2	-6.01	104.58	118.40
1	A	6	SER	O-C-N	6.01	129.79	123.06
1	A	12	ALA	N-CA-CB	5.89	120.03	110.77
1	A	120	ILE	CA-C-N	5.89	131.78	122.94
1	A	120	ILE	C-N-CA	5.89	131.78	122.94
1	A	70	ARG	CA-CB-CG	5.85	125.79	114.10
1	A	104	LEU	CB-CA-C	5.84	119.96	110.96
1	A	108	THR	CA-CB-CG2	5.84	120.42	110.50
1	A	26	PRO	CB-CA-C	5.83	120.13	111.62
1	A	167	SER	CA-C-N	-5.83	115.70	122.63
1	A	167	SER	C-N-CA	-5.83	115.70	122.63
1	A	133	MET	CA-C-O	-5.79	114.37	120.63
1	A	38	ARG	CB-CA-C	5.77	119.85	110.96
1	A	135	HIS	CB-CA-C	5.76	118.46	109.42
1	A	7	LEU	CA-C-O	-5.75	114.50	121.28
1	A	188	GLY	N-CA-C	-5.73	102.40	112.77
1	A	160	PHE	CA-C-O	-5.72	113.80	120.20
1	A	148	LYS	N-CA-C	-5.67	100.08	108.99
1	A	12	ALA	CA-C-N	-5.61	113.11	122.21
1	A	12	ALA	C-N-CA	-5.61	113.11	122.21
1	A	95	ALA	CA-C-O	-5.61	114.72	120.89
1	A	153	ASP	CB-CA-C	5.60	119.39	109.75
1	A	206	LEU	N-CA-CB	-5.59	101.00	110.50
1	A	114	SER	N-CA-C	-5.56	106.33	113.23
1	A	140	ARG	NE-CZ-NH1	-5.56	115.94	121.50
1	A	53	ASN	CA-C-N	-5.54	115.25	122.94
1	A	53	ASN	C-N-CA	-5.54	115.25	122.94
1	A	104	LEU	CA-C-N	5.53	127.96	120.38
1	A	104	LEU	C-N-CA	5.53	127.96	120.38
1	A	187	HIS	CB-CA-C	-5.52	100.16	109.72
1	A	38	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	128	LEU	CA-C-O	5.49	126.12	119.31
1	A	150	ILE	CB-CA-C	5.49	119.06	111.49
1	A	106	TYR	CB-CA-C	5.48	121.76	110.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	100	HIS	N-CA-CB	5.45	118.31	110.20
1	A	75	ARG	CD-NE-CZ	5.42	131.99	124.40
1	A	92	ILE	N-CA-C	-5.40	99.38	107.37
1	A	155	PHE	O-C-N	5.40	130.21	123.19
1	A	108	THR	CA-CB-OG1	-5.39	101.51	109.60
1	A	104	LEU	N-CA-C	-5.38	105.11	110.97
1	A	101	ALA	N-CA-C	-5.37	105.43	111.28
1	A	175	SER	N-CA-C	-5.36	105.55	111.71
1	A	189	LYS	CA-C-O	5.35	127.15	121.05
1	A	189	LYS	N-CA-C	5.32	118.61	110.20
1	A	129	TYR	O-C-N	5.29	127.80	122.09
1	A	165	TRP	CA-C-O	-5.26	113.74	119.95
1	A	75	ARG	CA-CB-CG	5.26	124.62	114.10
1	A	115	VAL	CA-C-O	5.25	126.05	120.48
1	A	203	THR	CA-CB-OG1	-5.24	101.73	109.60
1	A	28	LYS	CB-CA-C	-5.19	103.88	111.77
1	A	65	ILE	O-C-N	5.17	127.00	121.10
1	A	172	GLU	CB-CG-CD	-5.17	103.81	112.60
1	A	201	MET	O-C-N	5.17	129.32	123.27
1	A	109	TYR	CA-C-N	5.16	128.19	122.15
1	A	109	TYR	C-N-CA	5.16	128.19	122.15
1	A	55	VAL	CA-CB-CG1	5.16	119.17	110.40
1	A	39	VAL	CA-C-O	-5.15	115.92	121.27
1	A	96	LYS	CA-CB-CG	5.14	124.38	114.10
1	A	198	GLU	CB-CG-CD	5.13	121.33	112.60
1	A	56	LEU	CA-CB-CG	5.13	134.24	116.30
1	A	63	GLU	CA-CB-CG	5.11	124.31	114.10
1	A	173	LYS	CA-C-N	5.11	127.38	120.38
1	A	173	LYS	C-N-CA	5.11	127.38	120.38
1	A	156	PHE	CA-CB-CG	-5.07	108.73	113.80
1	A	12	ALA	N-CA-C	-5.07	100.03	108.34
1	A	87	ASP	O-C-N	5.05	128.55	122.79
1	A	7	LEU	O-C-N	5.03	128.89	123.10
1	A	192	GLU	CG-CD-OE1	5.02	129.96	118.40
1	A	58	GLY	N-CA-C	-5.02	105.03	113.02
1	A	169	TRP	O-C-N	5.02	128.94	123.22
1	A	151	HIS	CA-C-N	5.00	130.45	122.59
1	A	151	HIS	C-N-CA	5.00	130.45	122.59
1	A	180	TRP	CB-CA-C	5.00	118.80	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	PHE	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1686	0	1693	99	1
2	A	48	0	25	4	0
3	A	33	0	20	5	0
4	A	48	0	0	5	0
All	All	1815	0	1738	100	1

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 29.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:HB3	1:A:150:ILE:HD11	1.30	1.07
1:A:7:LEU:HB3	1:A:138:LEU:HD23	1.39	1.00
1:A:150:ILE:HD12	1:A:150:ILE:N	1.92	0.84
1:A:46:PHE:O	1:A:47:ASP:CG	2.20	0.84
1:A:122:VAL:HG13	1:A:128:LEU:HD13	1.61	0.83
1:A:150:ILE:HD12	1:A:150:ILE:H	1.47	0.79
1:A:189:LYS:HB2	4:A:245:HOH:O	1.83	0.77
1:A:86:LEU:O	1:A:86:LEU:HD22	1.86	0.76
1:A:81:THR:HG23	1:A:84:GLU:HB2	1.68	0.75
1:A:82:ARG:HG3	2:A:207:NAP:H2A	1.67	0.74
1:A:104:LEU:C	1:A:104:LEU:HD12	2.12	0.74
1:A:46:PHE:O	1:A:47:ASP:OD1	2.05	0.73
1:A:28:LYS:CG	1:A:28:LYS:O	2.34	0.73
1:A:46:PHE:O	1:A:47:ASP:CB	2.37	0.72
1:A:175:SER:HB3	4:A:242:HOH:O	1.90	0.72
1:A:122:VAL:HG13	1:A:128:LEU:CD1	2.19	0.72
1:A:33:ILE:CG2	3:A:307:MTX:HB2	2.21	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:CB	1:A:150:ILE:HD11	2.16	0.70
1:A:135:HIS:HD2	1:A:137:LYS:H	1.40	0.70
1:A:38:ARG:NH2	1:A:185:VAL:HG22	2.07	0.69
1:A:186:PRO:HB2	1:A:190:ILE:HD11	1.75	0.69
1:A:122:VAL:CG1	1:A:128:LEU:HD13	2.25	0.67
1:A:45:THR:HA	1:A:48:SER:OG	1.96	0.66
1:A:81:THR:CG2	1:A:84:GLU:HB2	2.27	0.64
1:A:33:ILE:HG23	3:A:307:MTX:HB2	1.80	0.64
1:A:86:LEU:CD1	1:A:86:LEU:H	2.11	0.63
1:A:46:PHE:O	1:A:47:ASP:HB3	1.98	0.63
1:A:163:LYS:O	1:A:166:SER:OG	2.12	0.62
1:A:86:LEU:H	1:A:86:LEU:HD12	1.64	0.62
1:A:17:TYR:OH	1:A:162:ASP:OD1	2.14	0.61
1:A:82:ARG:CG	2:A:207:NAP:H2A	2.31	0.61
1:A:173:LYS:HG2	4:A:238:HOH:O	2.00	0.61
1:A:84:GLU:HG3	1:A:94:SER:OG	2.01	0.60
1:A:5:LYS:HE3	1:A:118:ASN:O	2.01	0.60
1:A:55:VAL:HG22	1:A:123:ILE:HG21	1.82	0.60
1:A:3:GLN:HG2	1:A:137:LYS:HG3	1.83	0.60
1:A:93:HIS:NE2	1:A:109:TYR:OH	2.33	0.59
1:A:191:ASN:HA	1:A:195:PHE:O	2.03	0.59
1:A:7:LEU:CB	1:A:138:LEU:HD23	2.24	0.58
1:A:110:GLY:O	1:A:113:SER:N	2.37	0.57
1:A:20:GLY:HA3	2:A:207:NAP:O3D	2.04	0.56
1:A:148:LYS:C	1:A:150:ILE:HD12	2.30	0.56
1:A:28:LYS:O	1:A:28:LYS:HG3	2.05	0.55
1:A:187:HIS:CE1	4:A:243:HOH:O	2.59	0.55
1:A:173:LYS:O	1:A:176:ASP:HB2	2.06	0.55
1:A:3:GLN:HB3	1:A:137:LYS:HG3	1.90	0.54
1:A:86:LEU:CD1	1:A:86:LEU:N	2.71	0.54
1:A:43:VAL:HG22	1:A:118:ASN:OD1	2.08	0.53
1:A:54:VAL:HG22	1:A:76:ILE:HB	1.89	0.53
1:A:104:LEU:C	1:A:104:LEU:CD1	2.80	0.53
1:A:23:ASN:OD1	1:A:60:LYS:HE2	2.10	0.52
1:A:126:ALA:HB2	1:A:154:VAL:CG1	2.39	0.52
1:A:150:ILE:N	1:A:150:ILE:CD1	2.64	0.52
1:A:28:LYS:O	1:A:28:LYS:HG2	2.10	0.51
1:A:62:TRP:O	1:A:70:ARG:HD2	2.10	0.51
1:A:21:ARG:HB2	1:A:152:CYS:HA	1.93	0.50
1:A:47:ASP:C	1:A:49:PHE:H	2.18	0.50
1:A:29:LEU:HB3	1:A:32:GLU:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:C	1:A:150:ILE:CD1	2.85	0.50
1:A:56:LEU:HD13	1:A:98:LEU:HD12	1.93	0.49
1:A:4:GLN:HE21	1:A:4:GLN:HA	1.77	0.49
1:A:150:ILE:H	1:A:150:ILE:CD1	2.23	0.49
1:A:182:GLY:O	1:A:183:THR:OG1	2.26	0.49
1:A:25:LEU:HD21	3:A:307:MTX:C7	2.43	0.48
1:A:110:GLY:O	1:A:112:GLU:N	2.46	0.48
1:A:38:ARG:NH2	1:A:184:LYS:O	2.42	0.48
1:A:81:THR:HG23	1:A:84:GLU:CB	2.41	0.47
1:A:140:ARG:HG3	1:A:203:THR:HG22	1.97	0.47
1:A:169:TRP:CZ2	1:A:204:ARG:HD2	2.49	0.47
1:A:172:GLU:OE2	1:A:203:THR:OG1	2.24	0.47
1:A:81:THR:OG1	2:A:207:NAP:O2X	2.19	0.46
1:A:174:HIS:CE1	1:A:178:GLU:OE2	2.67	0.46
3:A:307:MTX:H15	3:A:307:MTX:HM1	1.69	0.46
1:A:153:ASP:HB2	4:A:248:HOH:O	2.15	0.46
1:A:86:LEU:O	1:A:86:LEU:HD13	2.16	0.45
1:A:182:GLY:C	1:A:183:THR:OG1	2.60	0.45
1:A:62:TRP:CH2	1:A:70:ARG:HG2	2.52	0.45
1:A:110:GLY:C	1:A:112:GLU:N	2.74	0.45
1:A:174:HIS:HE1	1:A:178:GLU:OE2	2.01	0.44
1:A:135:HIS:CG	1:A:136:PRO:HD2	2.53	0.44
1:A:88:LEU:HD22	1:A:88:LEU:HA	1.77	0.43
1:A:113:SER:HB3	1:A:116:GLN:NE2	2.34	0.43
1:A:172:GLU:CA	1:A:172:GLU:OE1	2.66	0.42
1:A:47:ASP:C	1:A:49:PHE:N	2.77	0.42
1:A:174:HIS:O	1:A:177:LEU:HB3	2.20	0.42
1:A:177:LEU:C	1:A:177:LEU:HD23	2.44	0.42
1:A:110:GLY:O	1:A:113:SER:HB2	2.19	0.42
1:A:7:LEU:O	1:A:138:LEU:HD22	2.19	0.42
1:A:45:THR:O	1:A:48:SER:N	2.49	0.42
1:A:110:GLY:C	1:A:112:GLU:H	2.28	0.42
1:A:86:LEU:HD12	1:A:86:LEU:N	2.30	0.42
1:A:21:ARG:HA	1:A:153:ASP:OD1	2.20	0.42
1:A:25:LEU:HD21	3:A:307:MTX:H7	2.03	0.41
1:A:43:VAL:HG11	1:A:51:SER:HB2	2.02	0.41
1:A:4:GLN:HA	1:A:4:GLN:NE2	2.36	0.41
1:A:4:GLN:NE2	1:A:4:GLN:CA	2.84	0.41
1:A:62:TRP:CH2	1:A:92:ILE:HD13	2.56	0.41
1:A:86:LEU:HD13	1:A:86:LEU:C	2.46	0.41
1:A:62:TRP:CZ2	1:A:70:ARG:HG2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:OE1	1:A:172:GLU:HA	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLN:NE2	1:A:164:GLU:O[2_556]	2.19	0.01

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
1	A	204/206 (99%)	188 (92%)	15 (7%)	1 (0%)	24 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	SER

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	187/187 (100%)	161 (86%)	26 (14%)	3 7

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	3	GLN
1	A	4	GLN
1	A	6	SER
1	A	21	ARG
1	A	25	LEU
1	A	29	LEU
1	A	51	SER
1	A	52	MET
1	A	55	VAL
1	A	84	GLU
1	A	85	SER
1	A	86	LEU
1	A	88	LEU
1	A	103	GLU
1	A	104	LEU
1	A	108	THR
1	A	112	GLU
1	A	113	SER
1	A	127	GLN
1	A	128	LEU
1	A	145	ILE
1	A	149	ASP
1	A	191	ASN
1	A	196	ASP
1	A	206	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	4	GLN
1	A	100	HIS
1	A	116	GLN
1	A	135	HIS
1	A	174	HIS
1	A	191	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](#)

2 ligands are modelled in this entry.

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
2	NAP	A	207	-	50,52,52	3.34	27 (54%)	71,80,80	2.29	24 (33%)
3	MTX	A	307	-	35,35,35	1.33	4 (11%)	47,49,49	1.84	8 (17%)

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
2	NAP	A	207	-	-	6/35/67/67	0/5/5/5
3	MTX	A	307	-	-	5/25/25/25	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	NAP	C4N-C3N	9.78	1.54	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	NAP	O4B-C4B	-8.32	1.26	1.45
2	A	207	NAP	P2B-O2B	7.54	1.72	1.59
2	A	207	NAP	C5N-C4N	6.73	1.50	1.38
2	A	207	NAP	O4D-C1D	6.13	1.48	1.40
2	A	207	NAP	C2N-N1N	5.85	1.41	1.35
2	A	207	NAP	C5A-C6A	5.56	1.56	1.41
2	A	207	NAP	C5A-C4A	-4.23	1.31	1.39
2	A	207	NAP	C3B-C4B	4.00	1.63	1.53
2	A	207	NAP	PA-O3	-3.77	1.55	1.59
2	A	207	NAP	C4A-N9A	-3.50	1.30	1.37
3	A	307	MTX	OE1-CD	3.41	1.33	1.22
3	A	307	MTX	C8A-N8	-3.30	1.32	1.37
2	A	207	NAP	O7N-C7N	-3.08	1.18	1.24
2	A	207	NAP	C5A-N7A	3.02	1.44	1.39
2	A	207	NAP	O3B-C3B	2.97	1.50	1.43
2	A	207	NAP	PA-O5B	2.94	1.70	1.59
2	A	207	NAP	C6N-C5N	-2.78	1.32	1.38
2	A	207	NAP	C6A-N1A	-2.71	1.28	1.35
3	A	307	MTX	O2-CT	-2.70	1.22	1.30
3	A	307	MTX	C2-NA2	-2.55	1.28	1.33
2	A	207	NAP	PN-O3	-2.51	1.56	1.59
2	A	207	NAP	C2N-C3N	-2.50	1.35	1.39
2	A	207	NAP	C6N-N1N	2.37	1.40	1.35
2	A	207	NAP	O2D-C2D	-2.37	1.37	1.43
2	A	207	NAP	C2D-C3D	2.34	1.59	1.53
2	A	207	NAP	P2B-O3X	-2.25	1.46	1.54
2	A	207	NAP	PN-O2N	-2.19	1.45	1.55
2	A	207	NAP	PN-O1N	-2.12	1.43	1.50
2	A	207	NAP	PA-O2A	-2.07	1.45	1.55
2	A	207	NAP	P2B-O2X	-2.04	1.47	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	207	NAP	C5N-C4N-C3N	-8.67	111.84	120.36
3	A	307	MTX	OE2-CD-OE1	-5.76	108.52	123.33
2	A	207	NAP	C4D-O4D-C1D	-5.54	104.85	109.92
2	A	207	NAP	P2B-O2B-C2B	5.50	138.12	123.43
3	A	307	MTX	C2-N1-C8A	4.89	120.76	115.48
2	A	207	NAP	O3B-C3B-C4B	-4.60	97.88	111.08
3	A	307	MTX	OE2-CD-CG	4.47	128.12	114.00
2	A	207	NAP	N6A-C6A-N1A	3.90	127.07	118.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	207	NAP	C2N-C3N-C4N	3.71	122.57	118.26
3	A	307	MTX	N1-C2-N3	-3.65	122.57	127.21
2	A	207	NAP	O3X-P2B-O2X	3.56	121.16	107.80
2	A	207	NAP	O5D-C5D-C4D	-3.55	96.92	108.99
2	A	207	NAP	O2A-PA-O3	3.40	116.45	107.27
2	A	207	NAP	C5A-C6A-N6A	-3.24	115.27	123.29
2	A	207	NAP	C4A-N9A-C8A	3.05	108.94	105.74
2	A	207	NAP	O2A-PA-O1A	3.01	126.44	112.44
2	A	207	NAP	N3A-C2A-N1A	2.96	133.06	128.58
2	A	207	NAP	O3-PN-O1N	2.84	119.26	110.70
3	A	307	MTX	N8-C8A-N1	2.84	118.87	115.77
2	A	207	NAP	C2D-C3D-C4D	-2.72	97.35	102.61
3	A	307	MTX	CG-CB-CA	2.58	117.92	113.16
2	A	207	NAP	C5A-N7A-C8A	-2.58	99.40	103.45
3	A	307	MTX	CT-CA-N	-2.53	104.70	110.57
2	A	207	NAP	C6N-C5N-C4N	2.50	123.05	119.45
2	A	207	NAP	C5B-C4B-C3B	-2.46	106.35	115.21
2	A	207	NAP	O5B-C5B-C4B	-2.44	100.67	108.99
2	A	207	NAP	C2B-C3B-C4B	-2.30	97.05	101.99
2	A	207	NAP	C3B-C2B-C1B	-2.27	98.47	102.81
2	A	207	NAP	O2B-C2B-C1B	-2.21	102.28	110.05
2	A	207	NAP	C4B-O4B-C1B	2.05	113.99	109.47
2	A	207	NAP	O2X-P2B-O2B	-2.03	97.95	105.85
3	A	307	MTX	CM-N10-C9	2.02	120.36	115.11

There are no chirality outliers.

All (11) torsion outliers are listed below:

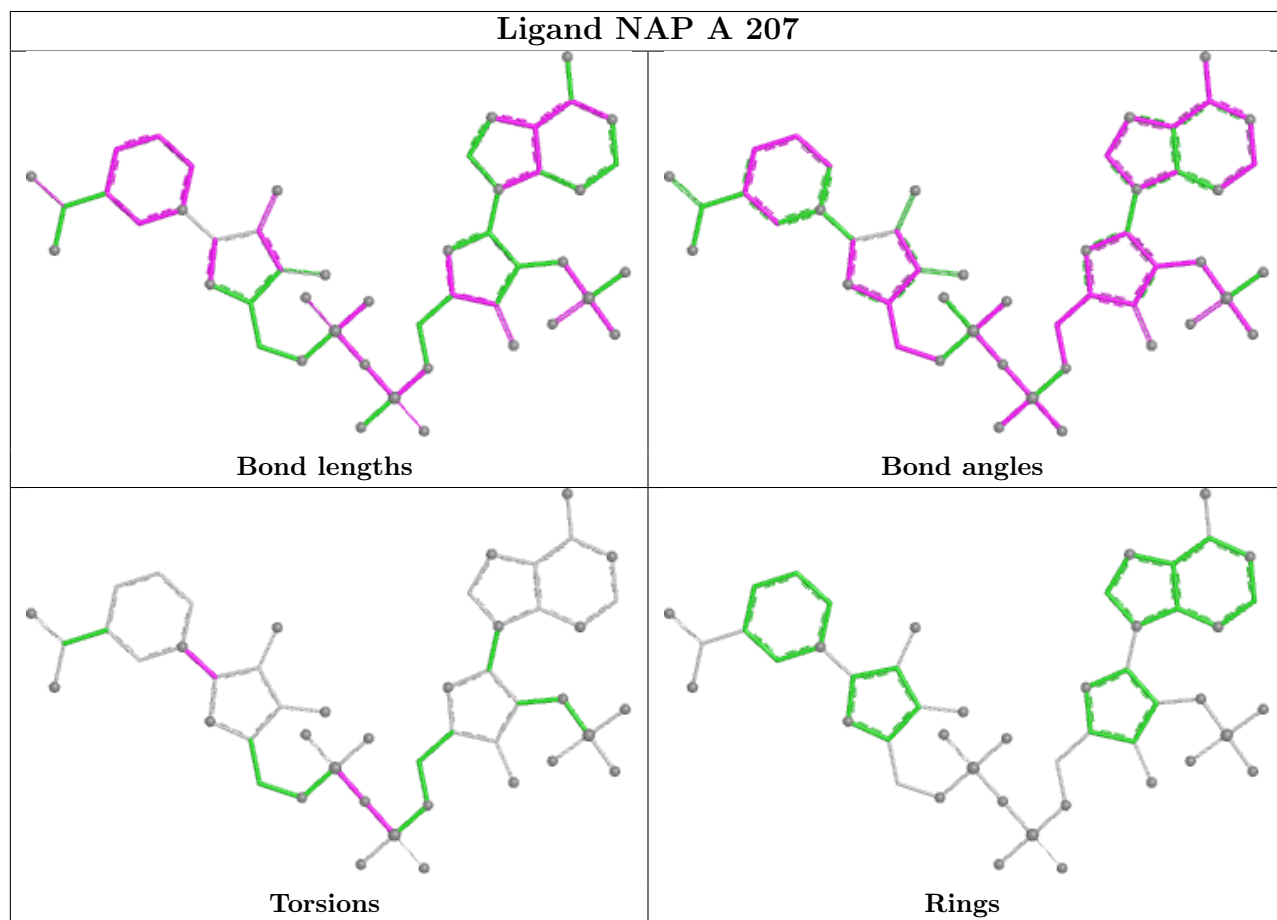
Mol	Chain	Res	Type	Atoms
2	A	207	NAP	O4D-C1D-N1N-C2N
2	A	207	NAP	O4D-C1D-N1N-C6N
3	A	307	MTX	N-CA-CB-CG
3	A	307	MTX	CT-CA-CB-CG
2	A	207	NAP	PN-O3-PA-O2A
2	A	207	NAP	PA-O3-PN-O1N
2	A	207	NAP	C2D-C1D-N1N-C2N
2	A	207	NAP	PN-O3-PA-O1A
3	A	307	MTX	C6-C9-N10-CM
3	A	307	MTX	OE1-CD-CG-CB
3	A	307	MTX	OE2-CD-CG-CB

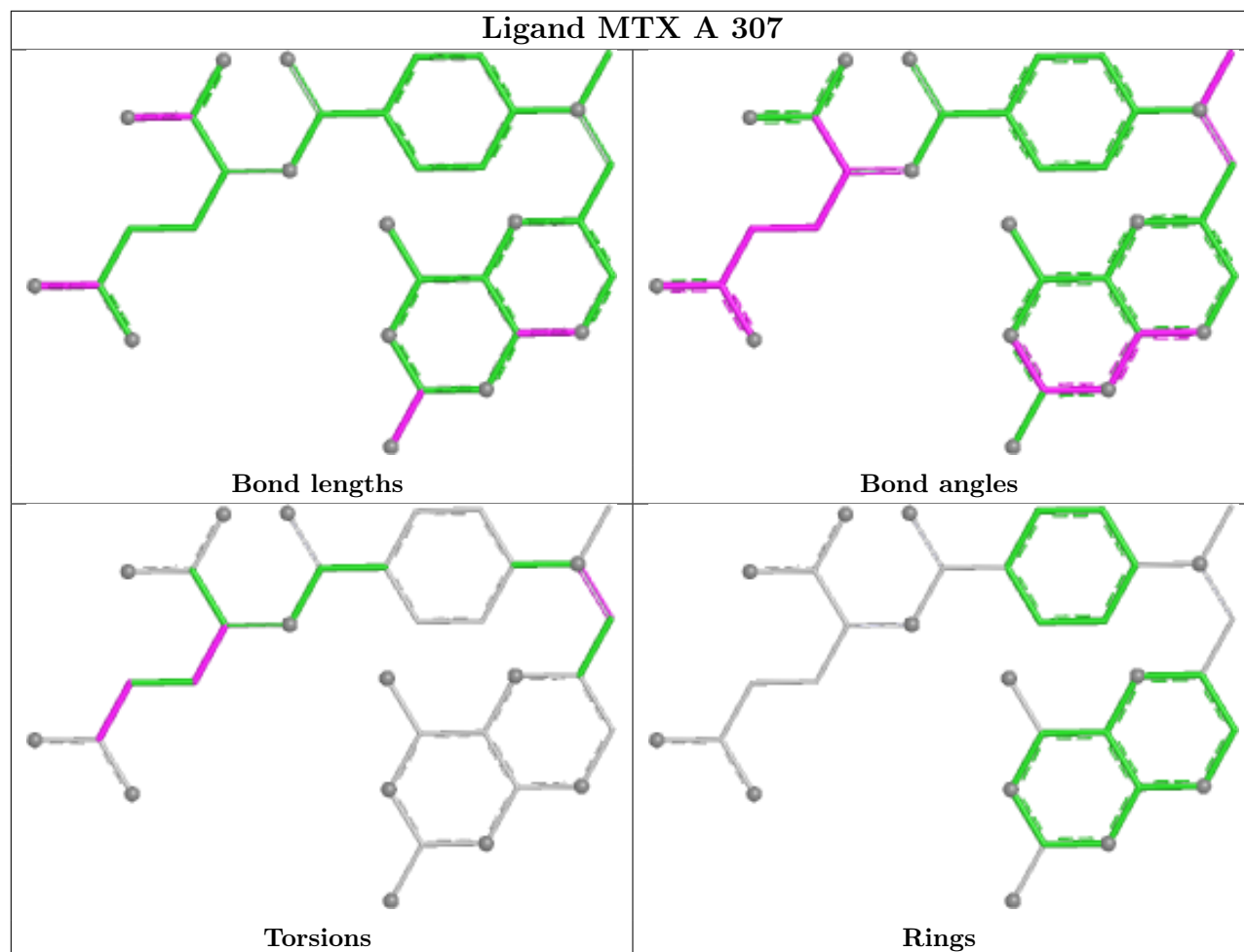
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	207	NAP	4	0
3	A	307	MTX	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.