



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:36 PM GMT

PDB ID : 4PGA
Title : GLUTAMINASE-ASPARAGINASE FROM PSEUDOMONAS 7A
Authors : Jakob, C.G.; Lewinski, K.; Lacount, M.W.; Roberts, J.; Lebioda, L.
Deposited on : 1997-01-14
Resolution : 1.70 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

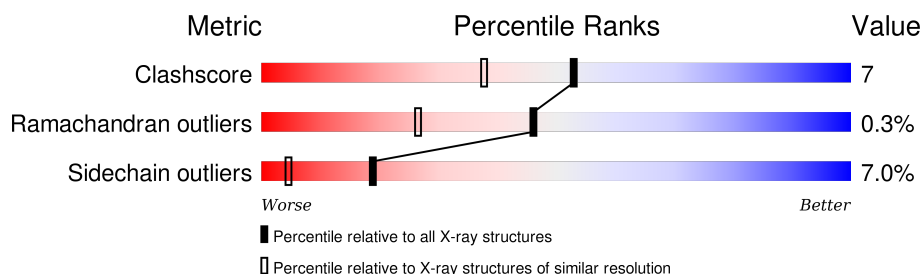
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)

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	A	337	
1	B	337	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5387 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 GLUTAMINASE-ASPARAGINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2485	1550	440	487	8			
1	B	330	Total	C	N	O	S	0	0	0
			2485	1550	440	487	8			

There are 24 discrepancies between the modelled and reference sequences:

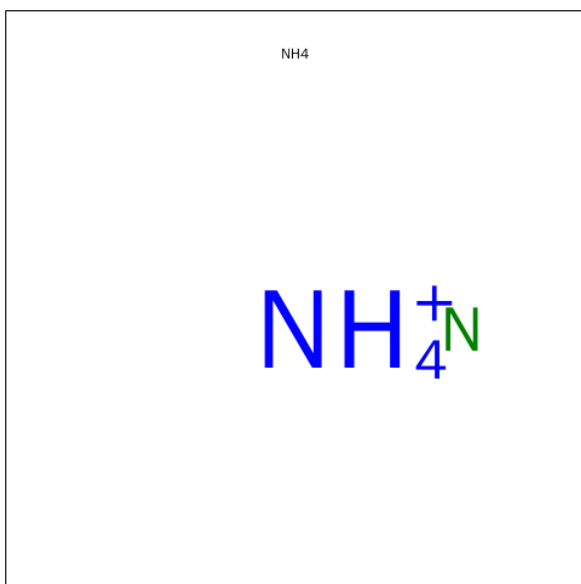
Chain	Residue	Modelled	Actual	Comment	Reference
A	111	ASN	ASP	CONFLICT	UNP P10182
A	113	VAL	THR	CONFLICT	UNP P10182
A	114	GLN	LEU	CONFLICT	UNP P10182
A	115	LYS	ASN	CONFLICT	UNP P10182
A	263	VAL	LEU	CONFLICT	UNP P10182
A	264	VAL	THR	CONFLICT	UNP P10182
A	269	GLN	THR	CONFLICT	UNP P10182
A	273	ASN	THR	CONFLICT	UNP P10182
A	317	ALA	VAL	CONFLICT	UNP P10182
A	318	MET	GLU	CONFLICT	UNP P10182
A	319	VAL	LEU	CONFLICT	UNP P10182
A	322	THR	VAL	CONFLICT	UNP P10182
B	111	ASN	ASP	CONFLICT	UNP P10182
B	113	VAL	THR	CONFLICT	UNP P10182
B	114	GLN	LEU	CONFLICT	UNP P10182
B	115	LYS	ASN	CONFLICT	UNP P10182
B	263	VAL	LEU	CONFLICT	UNP P10182
B	264	VAL	THR	CONFLICT	UNP P10182
B	269	GLN	THR	CONFLICT	UNP P10182
B	273	ASN	THR	CONFLICT	UNP P10182
B	317	ALA	VAL	CONFLICT	UNP P10182
B	318	MET	GLU	CONFLICT	UNP P10182
B	319	VAL	LEU	CONFLICT	UNP P10182
B	322	THR	VAL	CONFLICT	UNP P10182

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	N	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total N 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	177	Total O 177 177	0	0
4	B	228	Total O 228 228	0	0

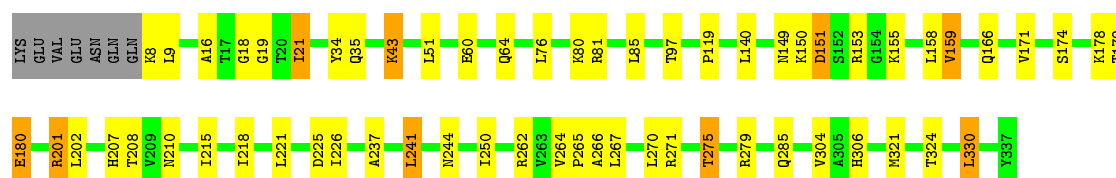
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

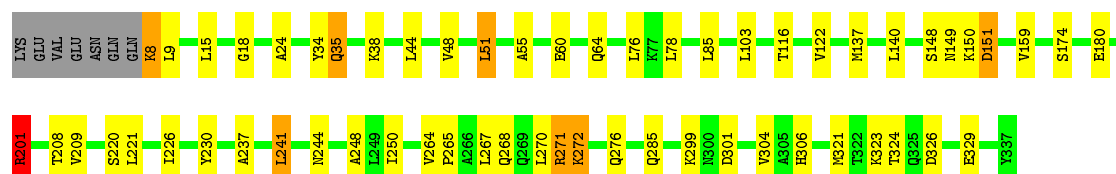
• Molecule 1: GLUTAMINASE-ASPARAGINASE

Chain A: 



• Molecule 1: GLUTAMINASE-ASPARAGINASE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	78.62Å 135.80Å 137.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70	Depositor
% Data completeness (in resolution range)	86.0 (10.00-1.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.199 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5387	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: NH4, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/2520	0.65	1/3413 (0.0%)
1	B	0.48	0/2520	0.65	1/3413 (0.0%)
All	All	0.48	0/5040	0.65	2/6826 (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	A	0	5
1	B	0	2
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	A	201	ARG	NE-CZ-NH2	-7.25	116.67	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	ARG	Sidechain
1	A	271	ARG	Sidechain
1	A	275	THR	Mainchain
1	A	279	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	34	TYR	Sidechain
1	B	201	ARG	Sidechain
1	B	34	TYR	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	A	2485	0	2505	33	1
1	B	2485	0	2505	36	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	177	0	0	5	1
4	B	228	0	0	5	0
All	All	5387	0	5010	66	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 7.

All (66) 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:B:122:VAL:O	1:B:159:VAL:HG13	1.71	0.88
1:B:35:GLN:HB2	1:B:38:LYS:HE2	1.58	0.85
1:B:24:ALA:HB3	1:B:38:LYS:HE3	1.66	0.76
1:B:116:THR:O	1:B:209:VAL:HG13	1.89	0.73
1:B:8:LYS:HD3	1:B:9:LEU:H	1.57	0.69
1:A:21:ILE:HG21	4:A:440:HOH:O	1.93	0.68
1:A:21:ILE:HD13	1:A:97:THR:HB	1.77	0.67
1:B:137:MET:HG2	4:B:495:HOH:O	1.94	0.67
1:B:116:THR:C	1:B:209:VAL:CG1	2.65	0.64
1:A:149:ASN:OD1	1:A:151:ASP:HB2	1.97	0.63
1:B:76:LEU:HD11	1:B:220:SER:HA	1.82	0.62
1:A:18:GLY:HA2	1:A:64:GLN:OE1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:HB	1:B:51:LEU:HD22	1.82	0.61
1:B:201:ARG:HD2	4:B:373:HOH:O	1.99	0.60
1:B:244:ASN:HB2	4:B:453:HOH:O	2.03	0.58
1:B:122:VAL:HB	1:B:159:VAL:HG22	1.87	0.57
1:B:18:GLY:HA2	1:B:64:GLN:OE1	2.05	0.57
1:A:150:LYS:HD3	1:A:150:LYS:O	2.06	0.56
1:B:149:ASN:OD1	1:B:151:ASP:HB2	2.05	0.56
1:A:237:ALA:O	1:A:241:LEU:HD22	2.09	0.52
1:A:262:ARG:NH1	1:A:262:ARG:HB3	2.25	0.52
1:B:237:ALA:O	1:B:241:LEU:HD22	2.09	0.52
1:A:60:GLU:OE2	1:A:81:ARG:HD3	2.10	0.52
1:B:264:VAL:HB	1:B:265:PRO:HD3	1.92	0.52
1:A:159:VAL:HG11	1:A:171:VAL:HG11	1.91	0.51
1:B:326:ASP:HB3	1:B:329:GLU:HB2	1.92	0.51
1:B:323:LYS:HB3	1:B:323:LYS:NZ	2.26	0.51
1:A:80:LYS:HD2	1:A:215:ILE:HG13	1.93	0.51
1:B:116:THR:C	1:B:209:VAL:HG13	2.29	0.51
1:A:266:ALA:O	1:A:270:LEU:HG	2.11	0.51
1:A:264:VAL:HB	1:A:265:PRO:HD3	1.92	0.50
1:B:248:ALA:HB2	1:B:276:GLN:HB2	1.92	0.50
1:A:226:ILE:HD12	1:B:230:TYR:CD1	2.47	0.49
1:B:55:ALA:HB2	1:B:148:SER:OG	2.14	0.48
1:A:174:SER:O	1:B:285:GLN:HB2	2.13	0.48
1:A:306:HIS:HE1	4:A:349:HOH:O	1.97	0.48
1:A:285:GLN:HB2	1:B:174:SER:O	2.14	0.48
1:B:268:GLN:O	1:B:272:LYS:HD3	2.13	0.48
1:A:43:LYS:HE2	1:A:43:LYS:HA	1.97	0.47
1:A:76:LEU:HD21	1:A:218:ILE:HG22	1.97	0.47
1:B:8:LYS:HD3	1:B:9:LEU:N	2.26	0.46
1:A:178:LYS:HE2	1:A:180:GLU:OE1	2.15	0.46
1:B:180:GLU:O	1:B:180:GLU:HG3	2.15	0.46
1:B:306:HIS:HD2	4:B:380:HOH:O	1.99	0.46
1:A:21:ILE:H	1:A:21:ILE:HG13	1.59	0.46
1:A:19:GLY:HA2	2:A:338:SO4:O1	2.16	0.45
1:B:321:MET:HA	1:B:324:THR:O	2.17	0.45
1:A:207:HIS:HE1	4:A:420:HOH:O	2.00	0.45
1:A:244:ASN:HB3	4:A:454:HOH:O	2.19	0.43
1:B:271:ARG:HH11	1:B:301:ASP:HB3	1.84	0.43
1:B:226:ILE:HG12	1:B:250:ILE:HB	2.01	0.42
1:B:180:GLU:HG2	4:B:496:HOH:O	2.19	0.42
1:B:248:ALA:CB	1:B:276:GLN:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ILE:HG12	1:A:250:ILE:HB	2.02	0.42
1:A:119:PRO:HD3	1:A:153:ARG:HG2	2.01	0.42
1:A:155:LYS:HE3	1:A:202:LEU:CD2	2.49	0.41
1:A:16:ALA:HA	1:A:97:THR:OG1	2.20	0.41
1:A:225:ASP:HB3	1:A:241:LEU:HG	2.02	0.41
1:B:103:LEU:HD21	1:B:159:VAL:HG11	2.02	0.41
1:A:324:THR:HG23	1:A:330:LEU:HD13	2.02	0.41
1:A:150:LYS:HE2	1:A:153:ARG:HD3	2.02	0.41
1:A:321:MET:HA	1:A:324:THR:O	2.21	0.41
1:B:15:LEU:HD23	1:B:60:GLU:HB3	2.02	0.40
1:B:9:LEU:HB3	1:B:55:ALA:HA	2.02	0.40
1:A:330:LEU:HA	1:A:330:LEU:HD12	1.93	0.40
1:A:166:GLN:NE2	4:A:377:HOH:O	2.54	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:179:THR:OG1	4:A:479:HOH:O[3_656]	1.84	0.36

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	328/337 (97%)	319 (97%)	8 (2%)	1 (0%)	46	26
1	B	328/337 (97%)	318 (97%)	9 (3%)	1 (0%)	46	26
All	All	656/674 (97%)	637 (97%)	17 (3%)	2 (0%)	46	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208	THR
1	A	208	THR

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	
1	A	265/272 (97%)	246 (93%)	19 (7%)	18	4
1	B	265/272 (97%)	247 (93%)	18 (7%)	20	5
All	All	530/544 (97%)	493 (93%)	37 (7%)	19	4

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	9	LEU
1	A	21	ILE
1	A	35	GLN
1	A	43	LYS
1	A	51	LEU
1	A	85	LEU
1	A	140	LEU
1	A	151	ASP
1	A	158	LEU
1	A	159	VAL
1	A	180	GLU
1	A	210	ASN
1	A	221	LEU
1	A	241	LEU
1	A	267	LEU
1	A	275	THR
1	A	304	VAL
1	A	330	LEU
1	B	8	LYS
1	B	35	GLN
1	B	44	LEU

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Mol	Chain	Res	Type
1	B	51	LEU
1	B	78	LEU
1	B	85	LEU
1	B	140	LEU
1	B	150	LYS
1	B	151	ASP
1	B	201	ARG
1	B	221	LEU
1	B	241	LEU
1	B	267	LEU
1	B	270	LEU
1	B	271	ARG
1	B	272	LYS
1	B	299	LYS
1	B	304	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	217	GLN
1	A	269	GLN
1	A	273	ASN
1	A	285	GLN
1	A	306	HIS
1	B	166	GLN
1	B	223	GLN
1	B	285	GLN
1	B	306	HIS
1	B	325	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are modelled with single atom - leaving 2 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	$\# Z > 2$
2	SO4	A	338	-	4,4,4	0.19	0	6,6,6	0.26	0
2	SO4	B	338	-	4,4,4	0.26	0	6,6,6	0.43	0

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	SO4	A	338	-	-	0/0/0/0	0/0/0/0
2	SO4	B	338	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	338	SO4	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.