



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:23 PM GMT

PDB ID : 1AIC
Title : STRUCTURAL BASIS FOR THE CATALYTIC ACTIVITY OF ASPARTATE AMINOTRANSFERASE K258H LACKING THE PYRIDOXAL-5'-PHOSPHATE BINDING LYSINE RESIDUE
Authors : Jaeger, J.; Jansonius, J.N.
Deposited on : 1994-05-10
Resolution : 2.40 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

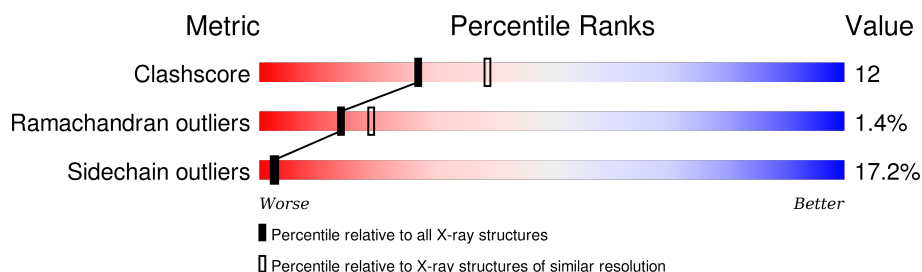
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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	396	 63% 23% 11% •
1	B	396	 67% 22% 8% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6182 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 ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3070	1936	537	584	13			
1	B	396	Total	C	N	O	S	0	0	0
			3070	1936	537	584	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	HIS	LYS	ENGINEERED MUTATION	UNP P00509
B	258	HIS	LYS	ENGINEERED MUTATION	UNP P00509

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



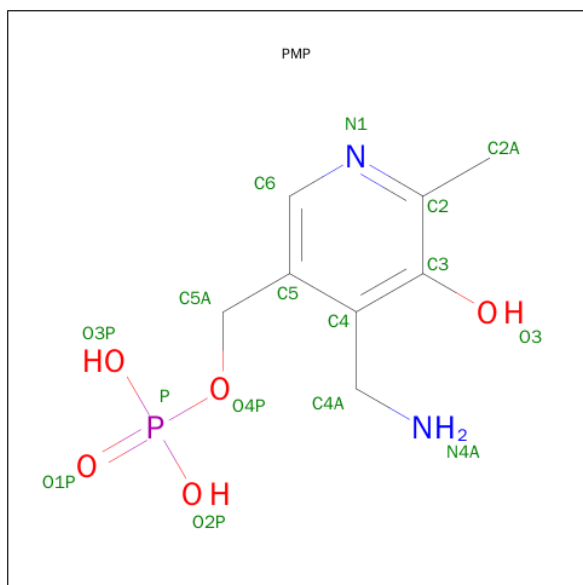
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C₈H₁₃N₂O₅P).



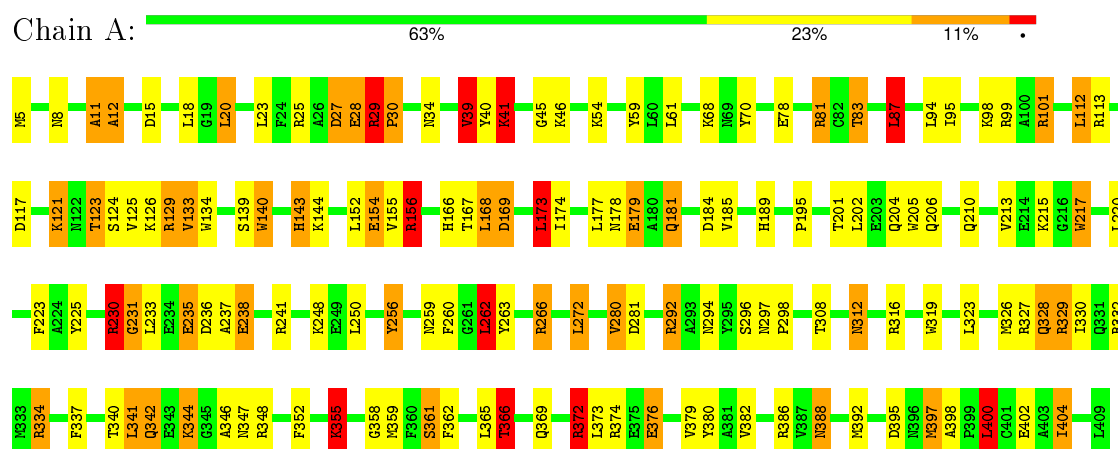
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

3 Residue-property plots

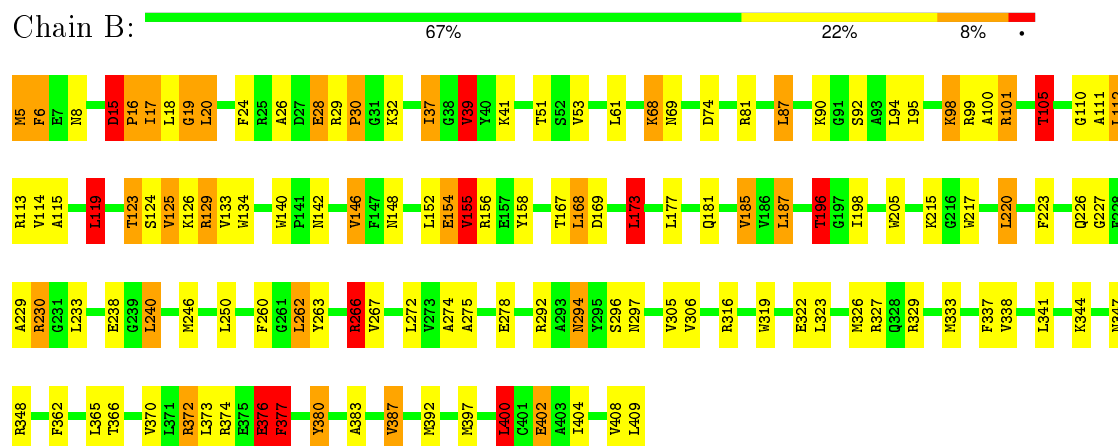
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ASPARTATE AMINOTRANSFERASE



• Molecule 1: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.20 Å 79.90 Å 89.60 Å 90.00° 119.10° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6182	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: PMP, 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	1.03	0/3132	1.91	87/4244 (2.0%)
1	B	1.28	9/3132 (0.3%)	1.82	68/4244 (1.6%)
All	All	1.16	9/6264 (0.1%)	1.87	155/8488 (1.8%)

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	2
1	B	0	3
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	GLY	N-CA	29.67	1.90	1.46
1	B	15	ASP	N-CA	21.56	1.89	1.46
1	B	16	PRO	C-N	16.30	1.71	1.34
1	B	17	ILE	CB-CG1	-15.23	1.11	1.54
1	B	15	ASP	C-N	-10.37	1.14	1.34
1	B	155	VAL	CA-CB	5.41	1.66	1.54
1	B	217	TRP	CG-CD2	-5.30	1.34	1.43
1	B	226	GLN	CA-CB	-5.23	1.42	1.53
1	B	376	GLU	CB-CG	5.08	1.61	1.52

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ARG	NE-CZ-NH2	-22.47	109.07	120.30
1	A	329	ARG	NE-CZ-NH2	-16.57	112.02	120.30
1	A	266	ARG	NE-CZ-NH1	15.43	128.01	120.30
1	B	266	ARG	NE-CZ-NH2	-14.25	113.17	120.30
1	A	113	ARG	NE-CZ-NH2	-12.61	114.00	120.30
1	B	316	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	B	377	PHE	CA-C-N	-11.54	93.13	116.20
1	B	17	ILE	CA-CB-CG1	10.96	131.82	111.00
1	B	230	ARG	NE-CZ-NH2	-10.77	114.91	120.30
1	A	319	TRP	CD1-CG-CD2	10.54	114.74	106.30
1	A	329	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	B	230	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	B	327	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	A	8	ASN	N-CA-CB	-9.94	92.72	110.60
1	A	217	TRP	CD1-CG-CD2	9.84	114.17	106.30
1	B	319	TRP	CD1-CG-CD2	9.82	114.16	106.30
1	A	8	ASN	CB-CA-C	9.58	129.57	110.40
1	B	327	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	A	372	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	B	372	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	B	266	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	A	366	THR	CA-CB-CG2	8.71	124.60	112.40
1	B	140	TRP	CD1-CG-CD2	8.35	112.98	106.30
1	A	178	ASN	CA-C-N	-8.26	99.03	117.20
1	A	169	ASP	CA-C-N	-8.25	99.04	117.20
1	B	377	PHE	O-C-N	8.23	137.19	123.20
1	A	355	LYS	CA-CB-CG	8.18	131.40	113.40
1	B	101	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	386	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	A	334	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	272	LEU	CA-CB-CG	7.99	133.68	115.30
1	B	319	TRP	CE2-CD2-CG	-7.89	100.99	107.30
1	A	329	ARG	CG-CD-NE	-7.87	95.27	111.80
1	A	328	GLN	CA-CB-CG	-7.84	96.15	113.40
1	A	319	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	A	59	TYR	CB-CG-CD1	-7.76	116.35	121.00
1	A	28	GLU	CA-CB-CG	7.75	130.45	113.40
1	A	319	TRP	CG-CD1-NE1	-7.72	102.38	110.10
1	B	319	TRP	CG-CD2-CE3	7.66	140.80	133.90
1	A	316	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	217	TRP	CE2-CD2-CG	-7.52	101.29	107.30
1	B	205	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	A	81	ARG	CA-CB-CG	7.41	129.70	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	B	5	MET	CA-C-N	7.38	133.45	117.20
1	B	5	MET	O-C-N	-7.34	110.95	122.70
1	B	217	TRP	CE2-CD2-CG	-7.32	101.45	107.30
1	A	11	ALA	N-CA-C	7.29	130.68	111.00
1	B	17	ILE	CB-CG1-CD1	7.22	134.11	113.90
1	B	196	THR	N-CA-CB	-7.21	96.59	110.30
1	B	205	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	A	280	VAL	CB-CA-C	-7.17	97.78	111.40
1	B	366	THR	CA-CB-CG2	-7.17	102.37	112.40
1	B	39	VAL	N-CA-CB	-7.05	95.99	111.50
1	B	173	LEU	CA-CB-CG	7.04	131.50	115.30
1	B	316	ARG	CG-CD-NE	-7.00	97.10	111.80
1	A	225	TYR	CB-CG-CD1	-6.94	116.84	121.00
1	A	41	LYS	N-CA-CB	-6.88	98.21	110.60
1	A	386	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	217	TRP	CG-CD1-NE1	-6.85	103.25	110.10
1	A	346	ALA	CA-C-N	-6.84	102.15	117.20
1	B	229	ALA	CA-C-N	6.78	132.11	117.20
1	A	230	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	A	205	TRP	CD1-CG-CD2	6.73	111.68	106.30
1	A	99	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	B	140	TRP	CE2-CD2-CG	-6.67	101.97	107.30
1	A	29	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	6	PHE	CB-CG-CD2	-6.64	116.16	120.80
1	A	205	TRP	CE2-CD2-CG	-6.62	102.01	107.30
1	A	319	TRP	CG-CD2-CE3	6.60	139.84	133.90
1	B	238	GLU	CA-CB-CG	6.56	127.83	113.40
1	B	319	TRP	CG-CD1-NE1	-6.52	103.58	110.10
1	B	125	VAL	CB-CA-C	-6.52	99.02	111.40
1	A	41	LYS	CB-CG-CD	-6.47	94.78	111.60
1	B	105	THR	N-CA-CB	-6.45	98.05	110.30
1	A	112	LEU	CA-CB-CG	6.42	130.07	115.30
1	A	238	GLU	CA-CB-CG	6.39	127.47	113.40
1	B	81	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	15	ASP	O-C-N	-6.38	108.98	121.10
1	A	29	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	374	ARG	CB-CA-C	-6.32	97.77	110.40
1	A	231	GLY	O-C-N	-6.19	112.80	122.70
1	A	140	TRP	CE2-CD2-CG	-6.18	102.36	107.30
1	A	250	LEU	CA-CB-CG	6.16	129.46	115.30
1	A	140	TRP	CD1-CG-CD2	6.14	111.22	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	VAL	CA-CB-CG1	-6.11	101.74	110.90
1	A	348	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	366	THR	CA-CB-OG1	-6.06	96.28	109.00
1	B	319	TRP	CB-CG-CD1	-6.02	119.17	127.00
1	B	154	GLU	CA-CB-CG	5.99	126.57	113.40
1	A	101	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	327	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	173	LEU	CA-CB-CG	5.93	128.93	115.30
1	A	292	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	15	ASP	N-CA-C	-5.88	95.11	111.00
1	B	217	TRP	CA-CB-CG	5.83	124.77	113.70
1	A	70	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	B	217	TRP	CD1-CG-CD2	5.80	110.94	106.30
1	B	217	TRP	NE1-CE2-CD2	5.79	113.09	107.30
1	A	133	VAL	O-C-N	5.79	131.97	122.70
1	B	272	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	119	LEU	CA-CB-CG	5.74	128.49	115.30
1	A	366	THR	N-CA-CB	-5.72	99.43	110.30
1	B	377	PHE	N-CA-C	5.71	126.42	111.00
1	B	6	PHE	CB-CA-C	-5.67	99.05	110.40
1	B	15	ASP	C-N-CD	-5.67	108.13	120.60
1	B	90	LYS	CA-C-N	5.67	127.53	116.20
1	A	87	LEU	CA-CB-CG	5.65	128.30	115.30
1	A	346	ALA	O-C-N	5.60	131.66	122.70
1	A	20	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	316	ARG	CG-CD-NE	-5.58	100.08	111.80
1	A	256	TYR	CB-CG-CD1	-5.58	117.66	121.00
1	B	229	ALA	O-C-N	-5.53	113.85	122.70
1	A	365	LEU	CB-CG-CD2	-5.52	101.61	111.00
1	B	87	LEU	CB-CG-CD2	-5.51	101.64	111.00
1	B	376	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	A	319	TRP	CB-CG-CD1	-5.50	119.85	127.00
1	B	380	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	A	40	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	A	262	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	154	GLU	CA-CB-CG	5.47	125.43	113.40
1	B	272	LEU	CB-CA-C	-5.45	99.84	110.20
1	A	25	ARG	CA-C-N	-5.45	105.21	117.20
1	A	39	VAL	N-CA-CB	-5.44	99.54	111.50
1	A	11	ALA	CB-CA-C	-5.42	101.97	110.10
1	B	400	LEU	CA-CB-CG	5.42	127.77	115.30
1	B	169	ASP	N-CA-C	-5.39	96.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	GLN	CB-CG-CD	5.36	125.52	111.60
1	A	156	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	230	ARG	CA-C-N	5.31	126.82	116.20
1	A	400	LEU	CA-CB-CG	5.31	127.50	115.30
1	B	68	LYS	CA-CB-CG	-5.30	101.75	113.40
1	A	397	MET	CG-SD-CE	-5.29	91.74	100.20
1	B	30	PRO	N-CA-C	5.29	125.84	112.10
1	A	113	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	387	VAL	N-CA-CB	-5.27	99.90	111.50
1	B	333	MET	CG-SD-CE	5.27	108.63	100.20
1	B	16	PRO	O-C-N	5.25	131.10	122.70
1	A	374	ARG	CA-CB-CG	5.23	124.91	113.40
1	A	12	ALA	N-CA-CB	5.23	117.42	110.10
1	B	374	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	129	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	213	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	A	365	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	179	GLU	N-CA-C	-5.13	97.16	111.00
1	B	272	LEU	CA-C-N	5.12	128.46	117.20
1	B	158	TYR	CA-CB-CG	5.11	123.11	113.40
1	B	217	TRP	CE2-CD2-CE3	5.10	124.82	118.70
1	A	173	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	A	113	ARG	CG-CD-NE	-5.08	101.13	111.80
1	A	281	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	236	ASP	O-C-N	-5.04	114.64	122.70
1	B	240	LEU	CA-CB-CG	5.04	126.88	115.30
1	B	39	VAL	CB-CA-C	5.01	120.92	111.40
1	A	382	VAL	CG1-CB-CG2	-5.01	102.89	110.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	GLY	Mainchain
1	A	329	ARG	Sidechain
1	B	134	TRP	Mainchain
1	B	15	ASP	Mainchain
1	B	376	GLU	Peptide

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	3070	0	3012	77	0
1	B	3070	0	3011	77	0
2	A	10	0	0	1	0
3	A	16	0	10	1	0
3	B	16	0	11	0	0
All	All	6182	0	6044	147	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 12.

All (147) 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:16:PRO:C	1:B:17:ILE:N	1.71	1.44
1:B:19:GLY:N	1:B:19:GLY:CA	1.90	1.34
1:B:15:ASP:CA	1:B:15:ASP:N	1.89	1.33
1:B:123:THR:HG22	1:B:125:VAL:H	0.99	1.11
1:B:123:THR:CG2	1:B:125:VAL:H	1.66	1.07
1:B:123:THR:HG22	1:B:125:VAL:N	1.81	0.95
1:A:294:ASN:HD21	1:B:294:ASN:HD21	1.11	0.93
1:A:123:THR:HG22	1:A:125:VAL:H	1.36	0.88
1:A:201:THR:H	1:A:204:GLN:HE21	1.23	0.86
1:A:126:LYS:HG2	1:A:126:LYS:O	1.78	0.82
1:A:123:THR:CG2	1:A:125:VAL:H	1.92	0.82
1:B:123:THR:HG21	1:B:125:VAL:HG23	1.63	0.81
1:A:29:ARG:HG2	1:A:29:ARG:HH11	1.44	0.81
1:A:123:THR:HG23	1:A:124:SER:H	1.46	0.79
1:B:123:THR:CG2	1:B:124:SER:N	2.48	0.77
1:A:266:ARG:HD2	1:B:297:ASN:O	1.88	0.74
1:A:123:THR:CG2	1:A:124:SER:N	2.52	0.71
1:B:344:LYS:HD2	1:B:402:GLU:HA	1.73	0.71
1:A:15:ASP:HB3	1:A:18:LEU:HB2	1.73	0.70
1:A:168:LEU:HD21	1:A:173:LEU:HD23	1.71	0.70
1:A:39:VAL:HG21	1:B:69:ASN:ND2	2.06	0.70
1:B:123:THR:HG23	1:B:124:SER:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:HG23	1:A:124:SER:N	2.07	0.67
1:A:29:ARG:NH1	1:A:29:ARG:HG2	2.07	0.67
1:B:337:PHE:HD1	1:B:397:MET:HE2	1.60	0.67
1:B:126:LYS:C	1:B:129:ARG:HG3	2.15	0.67
1:A:297:ASN:O	1:B:266:ARG:HD2	1.95	0.67
1:B:167:THR:HG22	1:B:168:LEU:H	1.59	0.66
1:B:105:THR:HG21	1:B:111:ALA:HB2	1.79	0.65
1:A:328:GLN:O	1:A:332:ARG:HD3	1.97	0.65
1:B:260:PHE:HB3	1:B:262:LEU:HD22	1.78	0.64
1:B:123:THR:HG23	1:B:124:SER:H	1.62	0.64
1:B:15:ASP:HB3	1:B:18:LEU:HB2	1.79	0.64
1:B:15:ASP:C	1:B:15:ASP:N	2.52	0.62
1:A:230:ARG:CG	1:A:235:GLU:HB3	2.30	0.62
1:B:16:PRO:CA	1:B:17:ILE:N	2.60	0.62
1:B:123:THR:CG2	1:B:125:VAL:N	2.51	0.61
1:A:337:PHE:HD1	1:A:397:MET:HE2	1.66	0.61
1:A:294:ASN:HD21	1:B:294:ASN:ND2	1.92	0.61
1:B:126:LYS:C	1:B:129:ARG:CG	2.69	0.61
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.83	0.60
1:A:41:LYS:HD3	1:A:45:GLY:HA2	1.82	0.60
1:A:366:THR:HG22	1:A:369:GLN:H	1.67	0.60
1:B:168:LEU:HD21	1:B:173:LEU:HD23	1.84	0.58
1:B:227:GLY:HA3	1:B:323:LEU:HD21	1.85	0.58
1:A:41:LYS:CD	1:A:45:GLY:HA2	2.33	0.57
1:B:99:ARG:HD3	1:B:275:ALA:O	2.03	0.57
1:B:397:MET:HE3	1:B:397:MET:HA	1.87	0.57
1:B:337:PHE:HB2	1:B:392:MET:HE1	1.88	0.56
1:B:99:ARG:HD2	1:B:274:ALA:O	2.06	0.56
1:A:133:VAL:HB	1:A:185:VAL:HB	1.87	0.56
1:B:39:VAL:HG22	1:B:263:TYR:CE1	2.41	0.56
1:B:126:LYS:O	1:B:126:LYS:CG	2.53	0.55
1:B:16:PRO:C	1:B:17:ILE:CA	2.71	0.55
1:A:126:LYS:CG	1:A:126:LYS:O	2.53	0.55
1:B:20:LEU:HD12	1:B:380:TYR:HD2	1.73	0.53
1:A:263:TYR:HB2	1:B:68:LYS:O	2.07	0.53
1:A:39:VAL:HG22	1:A:263:TYR:CZ	2.44	0.52
1:A:334:ARG:NH2	1:A:361:SER:OG	2.41	0.52
1:A:292:ARG:HA	1:A:296:SER:HA	1.91	0.52
1:B:133:VAL:HB	1:B:185:VAL:HG22	1.92	0.52
1:A:78:GLU:HA	1:A:81:ARG:HG3	1.91	0.51
1:A:129:ARG:HD3	1:A:184:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:H	1:A:78:GLU:CD	2.14	0.51
1:B:142:ASN:O	1:B:146:VAL:HG13	2.11	0.51
1:B:123:THR:CG2	1:B:125:VAL:HG23	2.38	0.51
1:B:187:LEU:HD12	1:B:220:LEU:HG	1.92	0.50
1:B:129:ARG:HA	1:B:154:GLU:O	2.12	0.50
1:B:370:VAL:HG21	1:B:383:ALA:HA	1.93	0.50
1:A:117:ASP:O	1:A:121:LYS:HG2	2.12	0.50
1:A:230:ARG:HG2	1:A:235:GLU:HB3	1.95	0.49
1:A:124:SER:O	1:A:125:VAL:C	2.48	0.49
1:B:196:THR:CG2	1:B:198:ILE:H	2.25	0.49
1:A:359:MET:HB3	1:A:388:ASN:ND2	2.27	0.49
1:B:196:THR:HG22	1:B:198:ILE:H	1.77	0.49
1:A:68:LYS:O	1:B:263:TYR:HB2	2.12	0.48
1:A:87:LEU:O	1:A:241:ARG:HD2	2.13	0.48
1:B:133:VAL:O	1:B:155:VAL:HA	2.12	0.48
1:A:201:THR:N	1:A:204:GLN:HE21	2.02	0.48
1:B:126:LYS:O	1:B:126:LYS:HG2	2.14	0.48
1:B:129:ARG:NH2	1:B:154:GLU:OE2	2.46	0.47
1:A:337:PHE:HD1	1:A:397:MET:CE	2.26	0.47
1:A:41:LYS:HE3	1:A:41:LYS:HB3	1.86	0.47
1:A:372:ARG:HD2	1:A:376:GLU:HG3	1.95	0.47
1:B:397:MET:HE1	1:B:400:LEU:HD13	1.95	0.47
1:A:373:LEU:HB3	1:A:379:VAL:HB	1.96	0.47
1:A:133:VAL:HA	1:A:185:VAL:O	2.13	0.46
1:B:196:THR:HG23	1:B:198:ILE:HB	1.96	0.46
1:A:39:VAL:HG21	1:B:69:ASN:HD21	1.77	0.46
1:A:144:LYS:HG3	1:A:155:VAL:HG21	1.97	0.46
1:A:34:ASN:HA	1:A:380:TYR:HB2	1.98	0.46
1:B:322:GLU:O	1:B:326:MET:HG3	2.15	0.46
1:B:37:ILE:HD12	1:B:41:LYS:HD2	1.97	0.46
1:A:248:LYS:HD3	1:A:248:LYS:HA	1.81	0.46
1:A:41:LYS:NZ	1:A:45:GLY:HA2	2.31	0.46
1:A:352:PHE:HA	1:A:355:LYS:HD3	1.98	0.46
1:A:392:MET:HG2	1:A:400:LEU:HD21	1.98	0.46
1:A:330:ILE:O	1:A:334:ARG:HG3	2.17	0.45
1:B:373:LEU:HD13	1:B:408:VAL:HG21	1.96	0.45
1:B:98:LYS:HE2	1:B:98:LYS:HA	1.99	0.45
1:B:177:LEU:HA	1:B:177:LEU:HD23	1.76	0.45
1:A:235:GLU:O	1:A:238:GLU:HG3	2.17	0.45
1:B:397:MET:CE	1:B:400:LEU:HD13	2.47	0.44
1:B:126:LYS:O	1:B:129:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:HD3	1:A:134:TRP:HE1	1.82	0.44
1:A:166:HIS:O	1:A:355:LYS:NZ	2.51	0.44
1:A:123:THR:CG2	1:A:124:SER:H	2.16	0.44
1:B:154:GLU:OE2	1:B:156:ARG:NH1	2.51	0.44
1:B:24:PHE:O	1:B:32:LYS:NZ	2.51	0.44
1:A:95:ILE:HD13	1:A:95:ILE:HG21	1.79	0.44
2:A:412:SO4:O4	3:A:411:PMP:N4A	2.47	0.44
1:A:27:ASP:OD2	1:A:29:ARG:HB2	2.18	0.43
1:A:340:THR:O	1:A:344:LYS:HG2	2.17	0.43
1:B:133:VAL:HA	1:B:185:VAL:O	2.18	0.43
1:A:83:THR:HB	1:A:256:TYR:OH	2.19	0.43
1:A:181:GLN:HG2	1:A:181:GLN:H	1.66	0.43
1:B:110:GLY:O	1:B:114:VAL:HG13	2.19	0.42
1:B:15:ASP:HA	1:B:16:PRO:HD3	1.65	0.42
1:B:292:ARG:HA	1:B:296:SER:HA	2.02	0.42
1:A:94:LEU:H	1:A:94:LEU:HD12	1.84	0.42
1:A:308:THR:O	1:A:312:ASN:ND2	2.52	0.42
1:B:267:VAL:HG11	1:B:306:VAL:HG21	2.01	0.42
1:A:237:ALA:O	1:A:241:ARG:HD3	2.20	0.42
1:B:404:ILE:O	1:B:409:LEU:HG	2.19	0.42
1:B:53:VAL:HG13	1:B:305:VAL:HG11	2.02	0.41
1:A:140:TRP:O	1:A:143:HIS:HB2	2.20	0.41
1:B:100:ALA:O	1:B:101:ARG:HD2	2.20	0.41
1:A:124:SER:C	1:A:125:VAL:O	2.55	0.41
1:B:112:LEU:HB3	1:B:146:VAL:HG21	2.01	0.41
1:A:323:LEU:HD12	1:A:326:MET:HE3	2.02	0.41
1:A:133:VAL:O	1:A:155:VAL:HA	2.21	0.41
1:B:115:ALA:O	1:B:119:LEU:HB2	2.20	0.41
1:B:39:VAL:HG22	1:B:263:TYR:CZ	2.55	0.41
1:A:177:LEU:O	1:A:217:TRP:HZ2	2.03	0.41
1:A:334:ARG:NH1	1:A:358:GLY:O	2.54	0.41
1:A:398:ALA:O	1:A:402:GLU:HG3	2.21	0.41
1:A:341:LEU:HD11	1:A:404:ILE:HG12	2.02	0.41
1:A:129:ARG:HE	1:A:156:ARG:HG3	1.86	0.41
1:B:37:ILE:O	1:B:37:ILE:HG12	2.21	0.40
1:A:237:ALA:HB3	1:A:241:ARG:NH1	2.36	0.40
1:A:133:VAL:CB	1:A:185:VAL:HB	2.51	0.40
1:A:139:SER:OG	1:A:189:HIS:HE1	2.05	0.40
1:B:344:LYS:HD3	1:B:344:LYS:O	2.21	0.40
1:B:98:LYS:CE	1:B:98:LYS:HA	2.51	0.40
1:B:28:GLU:OE1	1:B:32:LYS:NZ	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LYS:NZ	1:A:402:GLU:CD	2.75	0.40
1:B:95:ILE:HG21	1:B:95:ILE:HD13	1.84	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	
1	A	394/396 (100%)	364 (92%)	24 (6%)	6 (2%)	13	17
1	B	394/396 (100%)	373 (95%)	16 (4%)	5 (1%)	15	21
All	All	788/792 (100%)	737 (94%)	40 (5%)	11 (1%)	14	19

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	181	GLN
1	A	347	ASN
1	B	30	PRO
1	A	11	ALA
1	B	26	ALA
1	B	28	GLU
1	B	230	ARG
1	B	377	PHE
1	A	12	ALA
1	A	179	GLU

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	320/320 (100%)	263 (82%)	57 (18%)	2	2
1	B	320/320 (100%)	267 (83%)	53 (17%)	3	3
All	All	640/640 (100%)	530 (83%)	110 (17%)	2	3

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	20	LEU
1	A	23	LEU
1	A	27	ASP
1	A	28	GLU
1	A	29	ARG
1	A	30	PRO
1	A	39	VAL
1	A	41	LYS
1	A	46	LYS
1	A	54	LYS
1	A	61	LEU
1	A	83	THR
1	A	87	LEU
1	A	98	LYS
1	A	101	ARG
1	A	112	LEU
1	A	121	LYS
1	A	123	THR
1	A	143	HIS
1	A	152	LEU
1	A	154	GLU
1	A	156	ARG
1	A	167	THR
1	A	168	LEU
1	A	169	ASP
1	A	173	LEU

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Mol	Chain	Res	Type
1	A	174	ILE
1	A	195	PRO
1	A	202	LEU
1	A	206	GLN
1	A	210	GLN
1	A	215	LYS
1	A	220	LEU
1	A	223	PHE
1	A	230	ARG
1	A	233	LEU
1	A	235	GLU
1	A	259	ASN
1	A	262	LEU
1	A	272	LEU
1	A	280	VAL
1	A	298	PRO
1	A	312	ASN
1	A	341	LEU
1	A	342	GLN
1	A	344	LYS
1	A	355	LYS
1	A	361	SER
1	A	362	PHE
1	A	366	THR
1	A	372	ARG
1	A	376	GLU
1	A	388	ASN
1	A	395	ASP
1	A	400	LEU
1	A	404	ILE
1	B	5	MET
1	B	6	PHE
1	B	8	ASN
1	B	20	LEU
1	B	29	ARG
1	B	37	ILE
1	B	39	VAL
1	B	51	THR
1	B	61	LEU
1	B	74	ASP
1	B	87	LEU
1	B	92	SER

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Mol	Chain	Res	Type
1	B	94	LEU
1	B	98	LYS
1	B	105	THR
1	B	112	LEU
1	B	113	ARG
1	B	119	LEU
1	B	123	THR
1	B	146	VAL
1	B	148	ASN
1	B	152	LEU
1	B	155	VAL
1	B	168	LEU
1	B	173	LEU
1	B	181	GLN
1	B	185	VAL
1	B	187	LEU
1	B	196	THR
1	B	215	LYS
1	B	220	LEU
1	B	223	PHE
1	B	233	LEU
1	B	240	LEU
1	B	246	MET
1	B	250	LEU
1	B	262	LEU
1	B	266	ARG
1	B	278	GLU
1	B	294	ASN
1	B	329	ARG
1	B	338	VAL
1	B	341	LEU
1	B	347	ASN
1	B	348	ARG
1	B	362	PHE
1	B	365	LEU
1	B	372	ARG
1	B	376	GLU
1	B	377	PHE
1	B	387	VAL
1	B	400	LEU
1	B	402	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	189	HIS
1	A	204	GLN
1	A	226	GLN
1	A	258	HIS
1	A	259	ASN
1	A	312	ASN
1	A	388	ASN
1	B	69	ASN
1	B	148	ASN
1	B	226	GLN
1	B	247	HIS
1	B	294	ASN
1	B	335	GLN
1	B	342	GLN
1	B	347	ASN
1	B	356	GLN
1	B	357	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	PMP	A	411	-	16,16,16	2.02	4 (25%)	20,23,23	1.82	5 (25%)
2	SO4	A	412	-	4,4,4	1.91	2 (50%)	6,6,6	0.96	0
2	SO4	A	413	-	4,4,4	1.68	1 (25%)	6,6,6	0.70	0
3	PMP	B	411	-	16,16,16	2.57	4 (25%)	20,23,23	1.52	4 (20%)

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
3	PMP	A	411	-	-	0/8/8/8	0/1/1/1
2	SO4	A	412	-	-	0/0/0/0	0/0/0/0
2	SO4	A	413	-	-	0/0/0/0	0/0/0/0
3	PMP	B	411	-	-	0/8/8/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	411	PMP	C3-C2	-7.21	1.35	1.40
3	A	411	PMP	C3-C2	-5.48	1.37	1.40
3	B	411	PMP	C4A-C4	-5.03	1.34	1.51
3	A	411	PMP	C4A-C4	-3.37	1.40	1.51
3	A	411	PMP	O4P-C5A	-3.05	1.31	1.44
3	B	411	PMP	P-O2P	-2.44	1.45	1.54
3	B	411	PMP	O4P-C5A	-2.10	1.35	1.44
3	A	411	PMP	P-O2P	-2.02	1.47	1.54
2	A	413	SO4	O2-S	2.64	1.56	1.47
2	A	412	SO4	O2-S	2.68	1.56	1.47
2	A	412	SO4	O4-S	2.73	1.57	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	411	PMP	C5-C6-N1	-3.03	118.60	123.86
3	A	411	PMP	C5-C6-N1	-2.32	119.83	123.86
3	A	411	PMP	O2P-P-O4P	2.30	113.20	106.56
3	B	411	PMP	O4P-P-O1P	2.40	113.24	107.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	411	PMP	O4P-C5A-C5	2.47	113.07	108.99
3	A	411	PMP	C6-C5-C4	2.49	119.95	118.09
3	A	411	PMP	O2P-P-O1P	2.54	118.74	110.58
3	B	411	PMP	C6-C5-C4	3.96	121.04	118.09
3	A	411	PMP	O4P-C5A-C5	5.86	118.68	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	411	PMP	1	0
2	A	412	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.