



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:11 PM GMT

PDB ID : 5AT1
Title : STRUCTURAL CONSEQUENCES OF EFFECTOR BINDING TO THE
T STATE OF ASPARTATE CARBAMOYLTRANSFERASE. CRYSTAL
STRUCTURES OF THE UNLIGATED AND ATP-, AND CTP-
COMPLEXED ENZYMES AT 2.6-ANGSTROMS RESOLUTION
Authors : Stevens, R.C.; Gouaux, J.E.; Lipscomb, W.N.
Deposited on : 1990-04-26
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

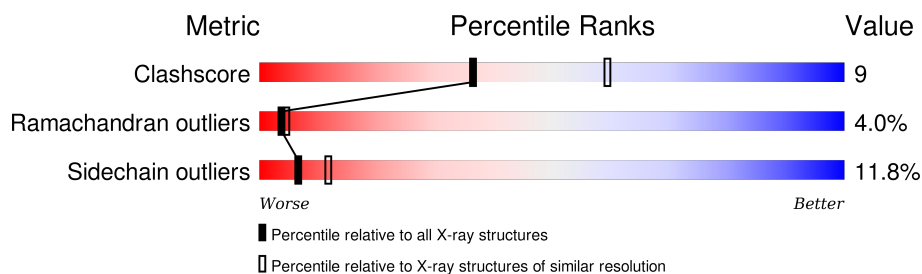
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	
1	C	310	
2	B	153	
2	D	153	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7166 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 CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	CONFLICT	UNP P0A786
A	147	GLN	GLU	CONFLICT	UNP P0A786
A	149	GLU	GLN	CONFLICT	UNP P0A786
A	196	GLU	GLN	CONFLICT	UNP P0A786
C	60	GLN	GLU	CONFLICT	UNP P0A786
C	147	GLN	GLU	CONFLICT	UNP P0A786
C	149	GLU	GLN	CONFLICT	UNP P0A786
C	196	GLU	GLN	CONFLICT	UNP P0A786

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

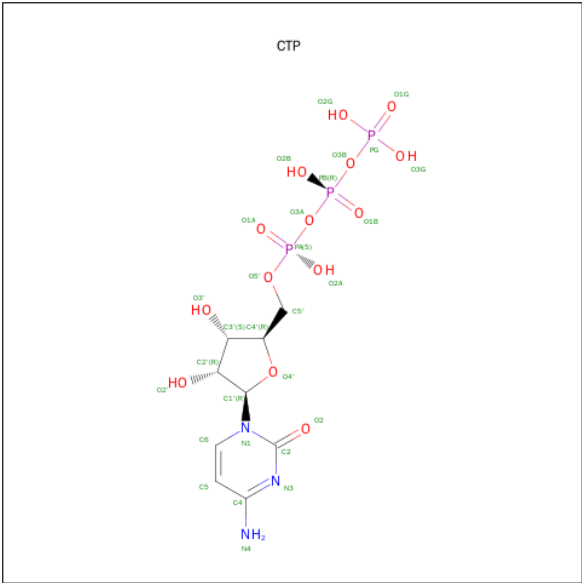
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	CONFLICT	UNP P0A7F3
D	8	GLY	GLN	CONFLICT	UNP P0A7F3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: C₉H₁₆N₃O₁₄P₃).



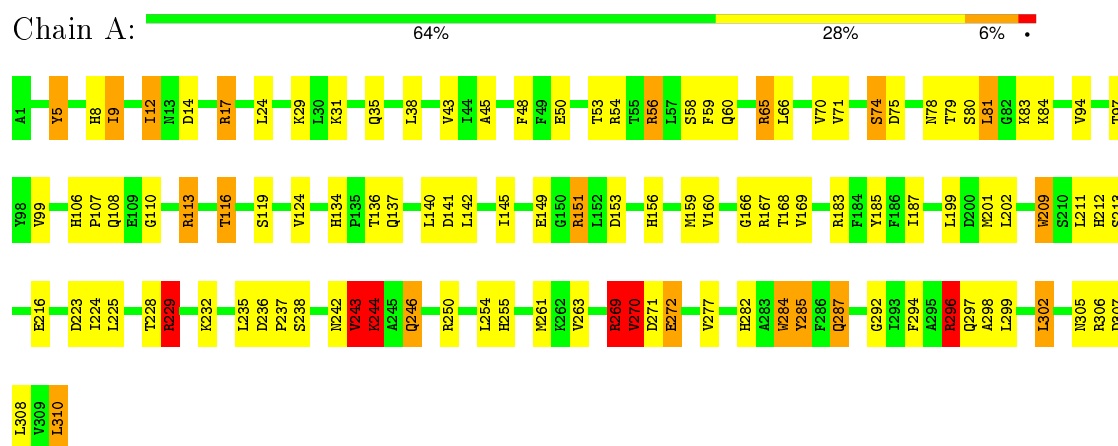
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	D	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

3 Residue-property plots

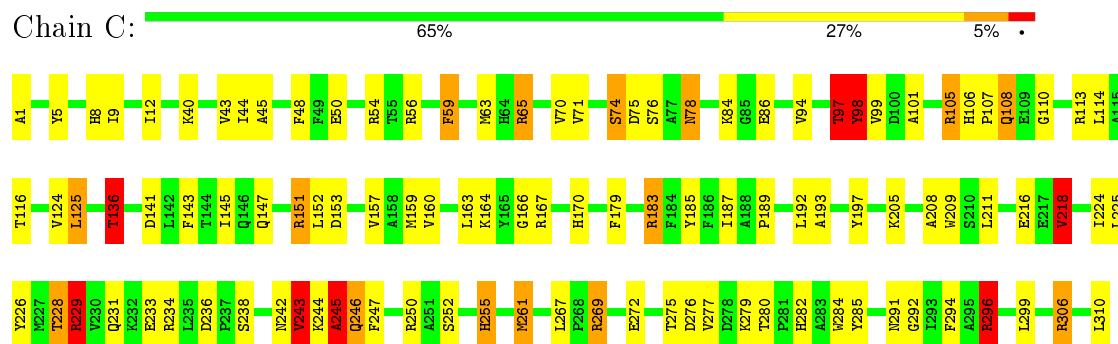
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

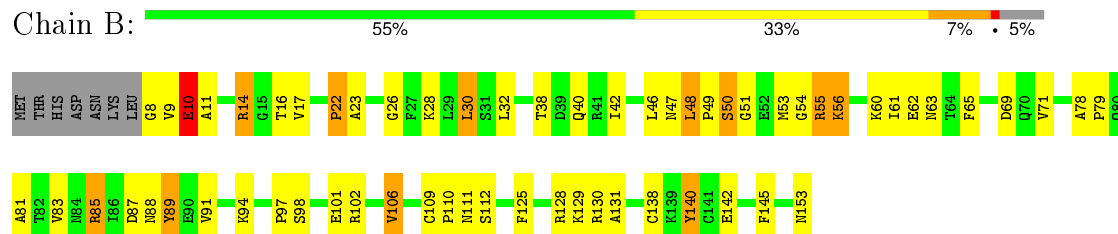
• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN



• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN



• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN



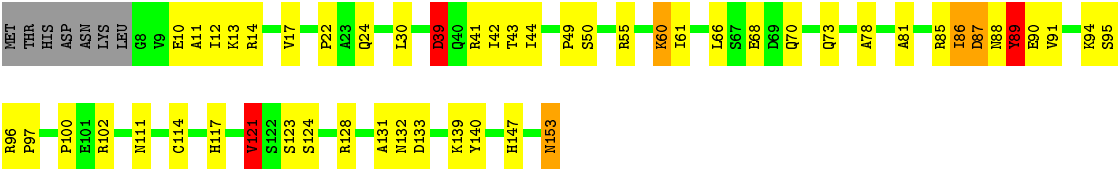
● Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN

Chain D:

61%

29%

• • 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.00 Å 122.00 Å 142.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7166	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: ZN, CTP

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	0.83	0/2461	1.61	39/3339 (1.2%)
1	C	0.88	0/2461	1.70	48/3339 (1.4%)
2	B	0.76	0/1155	1.52	11/1561 (0.7%)
2	D	0.78	1/1155 (0.1%)	1.49	11/1561 (0.7%)
All	All	0.83	1/7232 (0.0%)	1.61	109/9800 (1.1%)

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	C	0	4
2	B	0	2
2	D	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	60	LYS	CD-CE	-7.38	1.32	1.51

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	269	ARG	NE-CZ-NH2	14.58	127.59	120.30
1	C	54	ARG	NE-CZ-NH1	-12.86	113.87	120.30
1	A	269	ARG	NE-CZ-NH2	12.49	126.55	120.30
1	C	54	ARG	NE-CZ-NH2	11.78	126.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH1	-11.17	114.71	120.30
1	C	56	ARG	NE-CZ-NH1	-10.67	114.97	120.30
1	C	105	ARG	NE-CZ-NH2	10.05	125.33	120.30
1	C	269	ARG	NE-CZ-NH1	-9.98	115.31	120.30
1	C	98	TYR	CB-CG-CD2	-9.38	115.37	121.00
1	A	296	ARG	NE-CZ-NH2	8.77	124.69	120.30
1	C	113	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	A	43	VAL	CG1-CB-CG2	-8.43	97.41	110.90
1	C	113	ARG	NE-CZ-NH1	-8.05	116.28	120.30
1	C	167	ARG	CA-CB-CG	7.91	130.81	113.40
1	C	209	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	A	209	TRP	CD1-CG-CD2	7.84	112.57	106.30
2	B	62	GLU	CA-CB-CG	7.62	130.15	113.40
1	A	284	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	C	136	THR	N-CA-CB	-7.56	95.94	110.30
1	C	56	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	C	284	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	A	65	ARG	NE-CZ-NH2	7.45	124.02	120.30
1	C	105	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	A	56	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	C	56	ARG	CG-CD-NE	-7.16	96.77	111.80
1	C	43	VAL	CG1-CB-CG2	-7.14	99.48	110.90
1	A	284	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	C	209	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	C	284	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	A	209	TRP	CE2-CD2-CG	-6.99	101.70	107.30
2	D	85	ARG	NE-CZ-NH1	-6.89	116.85	120.30
2	D	85	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	A	113	ARG	NE-CZ-NH2	6.85	123.72	120.30
1	A	56	ARG	NE-CZ-NH1	-6.73	116.93	120.30
1	A	5	TYR	CB-CG-CD2	-6.73	116.96	121.00
2	D	55	ARG	NE-CZ-NH2	6.55	123.58	120.30
1	A	285	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	C	97	THR	N-CA-CB	-6.37	98.20	110.30
2	B	140	TYR	CB-CG-CD2	-6.16	117.30	121.00
1	C	54	ARG	CB-CG-CD	-6.09	95.77	111.60
1	C	229	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	183	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	C	157	VAL	CG1-CB-CG2	-6.05	101.23	110.90
1	A	159	MET	CA-CB-CG	-5.95	103.18	113.30
1	A	243	VAL	CA-CB-CG1	-5.93	102.01	110.90
2	D	89	TYR	N-CA-C	5.87	126.86	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ARG	CA-CB-CG	5.87	126.30	113.40
1	A	244	LYS	CA-CB-CG	5.85	126.27	113.40
1	C	284	TRP	CG-CD2-CE3	5.84	139.15	133.90
2	B	89	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	C	218	VAL	CA-CB-CG2	-5.73	102.31	110.90
1	A	17	ARG	NE-CZ-NH1	-5.72	117.44	120.30
2	B	51	GLY	N-CA-C	-5.72	98.81	113.10
2	D	114	CYS	CA-CB-SG	5.70	124.25	114.00
1	C	284	TRP	CB-CG-CD1	-5.69	119.61	127.00
2	B	106	VAL	N-CA-CB	-5.62	99.13	111.50
1	C	183	ARG	NE-CZ-NH2	5.60	123.10	120.30
2	D	153	ASN	N-CA-C	5.60	126.11	111.00
1	C	125	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	216	GLU	CA-CB-CG	5.54	125.58	113.40
2	B	85	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	201	MET	CG-SD-CE	-5.53	91.35	100.20
1	C	243	VAL	N-CA-C	-5.51	96.12	111.00
1	A	81	LEU	CA-CB-CG	5.51	127.97	115.30
1	C	40	LYS	CA-CB-CG	5.50	125.50	113.40
1	A	307	ASP	N-CA-C	-5.49	96.17	111.00
1	C	193	ALA	CB-CA-C	-5.45	101.92	110.10
1	A	229	ARG	CA-CB-CG	5.44	125.37	113.40
1	A	14	ASP	CA-CB-CG	5.42	125.32	113.40
1	C	245	ALA	N-CA-C	-5.39	96.43	111.00
1	A	250	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	C	183	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	C	228	THR	CA-CB-CG2	5.36	119.90	112.40
2	B	128	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	A	185	TYR	CB-CG-CD1	-5.34	117.79	121.00
2	B	54	GLY	N-CA-C	-5.33	99.78	113.10
1	C	71	VAL	O-C-N	-5.32	114.16	123.20
1	C	261	MET	CA-CB-CG	5.30	122.32	113.30
1	C	255	HIS	CA-CB-CG	-5.30	104.58	113.60
2	D	86	ILE	N-CA-C	-5.29	96.72	111.00
2	B	10	GLU	CA-C-N	5.29	128.83	117.20
1	A	183	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	A	229	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	A	65	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	A	116	THR	CA-CB-OG1	-5.25	97.97	109.00
1	C	116	THR	N-CA-CB	-5.25	100.33	110.30
1	A	71	VAL	CA-C-N	5.23	126.67	116.20
1	C	164	LYS	CB-CG-CD	-5.20	98.08	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	TRP	CG-CD1-NE1	-5.19	104.91	110.10
2	B	102	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	C	159	MET	CA-CB-CG	5.17	122.08	113.30
1	A	116	THR	CA-CB-CG2	5.16	119.63	112.40
1	C	197	TYR	CB-CG-CD2	-5.16	117.90	121.00
2	D	39	ASP	CA-C-N	-5.16	105.84	117.20
1	A	14	ASP	CB-CA-C	-5.13	100.14	110.40
1	C	243	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	C	98	TYR	CG-CD1-CE1	-5.10	117.22	121.30
1	A	9	ILE	CG1-CB-CG2	-5.09	100.19	111.40
1	A	54	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	C	250	ARG	NE-CZ-NH2	5.08	122.84	120.30
2	D	153	ASN	CA-CB-CG	5.08	124.58	113.40
1	C	211	LEU	CA-CB-CG	5.07	126.96	115.30
2	D	102	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	C	284	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	C	296	ARG	NE-CZ-NH2	5.04	122.82	120.30
2	D	121	VAL	CA-CB-CG2	-5.02	103.37	110.90
2	B	9	VAL	N-CA-C	-5.01	97.46	111.00
1	A	250	ARG	NE-CZ-NH2	5.01	122.80	120.30
1	C	276	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	HIS	Sidechain
1	A	5	TYR	Sidechain
2	B	48	LEU	Peptide
2	B	89	TYR	Sidechain
1	C	226	TYR	Sidechain
1	C	255	HIS	Sidechain
1	C	294	PHE	Sidechain
1	C	98	TYR	Sidechain
2	D	89	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	2415	0	2422	40	0
1	C	2415	0	2422	43	0
2	B	1138	0	1154	30	0
2	D	1138	0	1154	25	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	29	0	12	7	0
4	D	29	0	11	6	0
All	All	7166	0	7175	135	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 9.

All (135) 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:136:THR:HB	1:A:296:ARG:HH21	1.35	0.90
1:C:136:THR:HG23	1:C:296:ARG:HH21	1.44	0.81
1:C:280:THR:HG22	1:C:282:HIS:H	1.53	0.73
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.71	0.73
2:D:60:LYS:NZ	4:D:155:CTP:O2	2.23	0.71
1:C:292:GLY:O	1:C:296:ARG:HB2	1.91	0.70
1:A:106:HIS:HD2	1:A:108:GLN:H	1.36	0.70
2:D:94:LYS:NZ	4:D:155:CTP:O2A	2.20	0.70
1:A:136:THR:HB	1:A:296:ARG:NH2	2.06	0.70
2:B:94:LYS:HE3	4:B:155:CTP:O2A	1.92	0.69
2:B:94:LYS:CE	4:B:155:CTP:O2A	2.41	0.68
1:C:94:VAL:O	1:C:97:THR:HB	1.96	0.65
2:B:17:VAL:HG21	4:B:155:CTP:O2	1.97	0.65
1:A:8:HIS:HD2	1:A:124:VAL:H	1.45	0.65
2:B:8:GLY:N	2:B:50:SER:HG	1.96	0.64
1:C:136:THR:HG23	1:C:296:ARG:NH2	2.12	0.64
1:A:94:VAL:O	1:A:97:THR:HG22	1.98	0.63
2:D:42:ILE:HG12	2:D:61:ILE:HG23	1.78	0.63
1:A:160:VAL:O	1:A:228:THR:HG22	1.99	0.63
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.79	0.63
2:B:48:LEU:O	2:B:55:ARG:HA	1.98	0.62
2:B:38:THR:HG22	2:B:40:GLN:H	1.65	0.61
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.82	0.61
1:A:261:MET:O	1:A:282:HIS:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ALA:HA	1:C:306:ARG:HD3	1.84	0.60
2:D:14:ARG:HG3	2:D:87:ASP:HA	1.83	0.60
1:C:9:ILE:HB	1:C:125:LEU:HD13	1.84	0.60
1:C:189:PRO:HG2	1:C:192:LEU:HD12	1.84	0.60
2:D:30:LEU:HD11	2:D:44:ILE:HD13	1.84	0.59
2:D:60:LYS:CE	4:D:155:CTP:O2	2.50	0.59
1:C:163:LEU:O	1:C:170:HIS:HE1	1.86	0.59
1:C:277:VAL:O	1:C:280:THR:HB	2.03	0.58
1:A:29:LYS:HD3	1:A:310:LEU:HB2	1.85	0.58
2:B:22:PRO:O	2:B:56:LYS:HA	2.03	0.58
1:A:270:VAL:HG13	1:A:271:ASP:H	1.69	0.58
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.19	0.58
1:C:151:ARG:HG3	1:C:153:ASP:O	2.03	0.57
1:A:229:ARG:NH1	1:A:270:VAL:HG11	2.20	0.56
2:B:71:VAL:HG13	2:B:83:VAL:HG21	1.86	0.56
1:A:254:LEU:HD11	1:A:277:VAL:HG13	1.87	0.55
1:A:187:ILE:HG13	1:A:212:HIS:HB2	1.89	0.55
1:C:50:GLU:HB2	1:C:107:PRO:HD3	1.88	0.55
1:C:145:ILE:HG23	1:C:224:ILE:HG13	1.89	0.54
1:C:261:MET:O	1:C:282:HIS:HD2	1.89	0.54
1:C:45:ALA:HB2	1:C:99:VAL:HG11	1.89	0.54
2:B:91:VAL:HG21	4:B:155:CTP:PA	2.48	0.53
2:D:81:ALA:O	2:D:97:PRO:HD3	2.09	0.52
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.92	0.52
4:D:155:CTP:H6	4:D:155:CTP:H5'1	1.74	0.52
2:D:133:ASP:HB2	2:D:147:HIS:CE1	2.45	0.52
1:C:152:LEU:HD23	1:C:179:PHE:CZ	2.44	0.52
1:A:209:TRP:HZ3	1:A:211:LEU:HG	1.75	0.52
2:B:14:ARG:HH21	2:B:63:ASN:HA	1.75	0.52
2:B:47:ASN:ND2	2:D:39:ASP:HA	2.25	0.51
1:C:48:PHE:O	1:C:74:SER:HA	2.10	0.50
1:A:142:LEU:HA	1:A:145:ILE:HD12	1.93	0.50
2:D:60:LYS:HE3	4:D:155:CTP:O2	2.12	0.50
2:D:124:SER:HB3	2:D:139:LYS:HB2	1.94	0.50
1:A:66:LEU:HG	1:A:297:GLN:HE21	1.77	0.49
2:D:14:ARG:HA	2:D:86:ILE:O	2.13	0.49
2:B:71:VAL:HG22	2:B:83:VAL:HG11	1.95	0.49
1:A:145:ILE:HG23	1:A:224:ILE:HG13	1.94	0.49
2:B:81:ALA:O	2:B:97:PRO:HD2	2.13	0.48
2:B:17:VAL:HG11	4:B:155:CTP:O3'	2.14	0.48
2:D:17:VAL:HG13	2:D:60:LYS:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:O	1:A:261:MET:HA	2.13	0.48
1:C:143:PHE:HD1	1:C:291:ASN:HB3	1.79	0.48
1:C:185:TYR:CD2	1:C:218:VAL:HG21	2.49	0.47
1:C:189:PRO:CG	1:C:192:LEU:HD12	2.45	0.47
2:B:109:CYS:HA	2:B:125:PHE:HZ	1.80	0.47
2:D:13:LYS:HD3	2:D:14:ARG:HB2	1.96	0.47
2:B:16:THR:OG1	2:B:65:PHE:HA	2.15	0.47
1:A:261:MET:O	1:A:282:HIS:CD2	2.65	0.47
1:C:160:VAL:HG22	1:C:187:ILE:HD13	1.96	0.47
2:D:111:ASN:O	2:D:117:HIS:HE1	1.99	0.46
1:C:106:HIS:HD2	1:C:108:GLN:H	1.63	0.46
1:A:140:LEU:HD22	1:A:292:GLY:HA2	1.96	0.46
1:C:75:ASP:OD2	1:C:78:ASN:HA	2.16	0.45
1:A:12:ILE:HA	1:A:12:ILE:HD13	1.75	0.45
2:B:60:LYS:NZ	4:B:155:CTP:O2'	2.50	0.45
1:A:31:LYS:HA	1:A:294:PHE:CE1	2.52	0.45
1:C:65:ARG:HH21	1:C:65:ARG:HD2	1.63	0.45
2:D:11:ALA:HB1	4:D:155:CTP:C4	2.52	0.45
2:B:138:CYS:O	2:B:142:GLU:HA	2.17	0.45
1:A:60:GLN:HG2	1:A:70:VAL:HG11	1.99	0.45
2:B:11:ALA:HB1	4:B:155:CTP:N4	2.31	0.45
2:D:66:LEU:HA	2:D:70:GLN:OE1	2.18	0.44
1:A:9:ILE:HG12	1:A:299:LEU:HD11	1.99	0.44
1:A:199:LEU:O	1:A:202:LEU:HB2	2.18	0.44
1:C:243:VAL:HG12	1:C:244:LYS:H	1.83	0.44
1:A:225:LEU:HD12	1:A:263:VAL:HG13	1.99	0.44
1:C:183:ARG:HG2	1:C:208:ALA:HB3	1.99	0.44
1:A:48:PHE:O	1:A:74:SER:HA	2.18	0.44
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.18	0.43
1:C:229:ARG:HA	1:C:272:GLU:OE2	2.18	0.43
1:A:110:GLY:HA3	2:B:140:TYR:HB3	2.00	0.43
1:A:38:LEU:HD21	1:A:308:LEU:HD11	1.99	0.43
2:B:55:ARG:HD3	2:B:55:ARG:H	1.83	0.43
2:D:133:ASP:HB2	2:D:147:HIS:HE1	1.83	0.43
1:C:245:ALA:O	1:C:246:GLN:HG2	2.18	0.43
2:D:17:VAL:HG22	2:D:60:LYS:HG2	2.01	0.43
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.54	0.43
1:C:141:ASP:O	1:C:145:ILE:HG13	2.19	0.43
2:B:14:ARG:NH2	2:B:63:ASN:HA	2.34	0.43
1:A:141:ASP:O	1:A:145:ILE:HG13	2.19	0.43
2:B:130:ARG:HH11	2:B:131:ALA:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:VAL:HG23	1:A:246:GLN:NE2	2.34	0.42
1:A:145:ILE:O	1:A:149:GLU:HG2	2.20	0.42
1:C:160:VAL:HG21	1:C:225:LEU:HD11	2.01	0.42
1:C:8:HIS:HD2	1:C:124:VAL:H	1.66	0.42
1:C:189:PRO:HD3	1:C:247:PHE:CD2	2.54	0.42
2:B:110:PRO:HD2	2:B:145:PHE:CD1	2.54	0.42
1:C:261:MET:O	1:C:282:HIS:CD2	2.71	0.42
1:C:44:ILE:HG23	1:C:101:ALA:HB3	2.02	0.42
1:A:298:ALA:O	1:A:302:LEU:HD12	2.19	0.42
1:A:151:ARG:NH2	1:A:153:ASP:O	2.53	0.42
1:C:205:LYS:HB3	1:C:205:LYS:HE2	1.82	0.42
2:D:111:ASN:O	2:D:117:HIS:CE1	2.73	0.41
1:C:110:GLY:HA2	2:D:140:TYR:O	2.19	0.41
2:B:109:CYS:SG	2:B:111:ASN:HB3	2.60	0.41
2:B:42:ILE:HG12	2:B:61:ILE:HG23	2.03	0.41
1:C:59:PHE:CE2	1:C:296:ARG:HG3	2.56	0.41
2:D:22:PRO:HD2	2:D:78:ALA:HB1	2.03	0.41
1:C:63:MET:SD	1:C:70:VAL:HG22	2.61	0.41
2:D:12:ILE:HD12	2:D:14:ARG:O	2.21	0.41
1:C:5:TYR:CE1	1:C:306:ARG:HG2	2.56	0.41
2:B:26:GLY:O	2:B:30:LEU:HD22	2.20	0.41
2:B:65:PHE:CD2	2:B:85:ARG:HG3	2.56	0.40
2:B:28:LYS:HE3	2:B:28:LYS:HB2	1.95	0.40
1:A:166:GLY:O	1:A:169:VAL:HG22	2.22	0.40
1:A:229:ARG:HH11	1:A:270:VAL:HG11	1.86	0.40
1:C:114:LEU:HD12	2:D:121:VAL:HG21	2.02	0.40
1:C:238:SER:O	1:C:242:ASN:HB3	2.21	0.40
1:C:246:GLN:OE1	1:C:246:GLN:HA	2.21	0.40
2:D:73:GLN:NE2	2:D:100:PRO:HG3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	308/310 (99%)	279 (91%)	20 (6%)	9 (3%)	6	9
1	C	308/310 (99%)	279 (91%)	20 (6%)	9 (3%)	6	9
2	B	144/153 (94%)	113 (78%)	21 (15%)	10 (7%)	1	1
2	D	144/153 (94%)	130 (90%)	6 (4%)	8 (6%)	2	2
All	All	904/926 (98%)	801 (89%)	67 (7%)	36 (4%)	4	4

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	LYS
2	B	50	SER
2	D	49	PRO
2	D	89	TYR
2	D	131	ALA
1	A	83	LYS
1	A	243	VAL
1	A	270	VAL
2	B	10	GLU
2	B	22	PRO
2	B	53	MET
1	C	76	SER
2	D	88	ASN
1	A	75	ASP
1	A	80	SER
2	B	129	LYS
1	C	275	THR
2	D	50	SER
1	A	242	ASN
1	A	246	GLN
2	B	14	ARG
2	B	23	ALA
1	C	78	ASN
1	C	86	GLU
1	C	245	ALA
1	C	246	GLN
2	D	68	GLU
1	A	306	ARG
1	C	166	GLY
1	C	267	LEU
2	D	24	GLN
2	B	78	ALA
1	C	243	VAL

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Mol	Chain	Res	Type
2	B	49	PRO
2	B	79	PRO
2	D	91	VAL

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	261/261 (100%)	223 (85%)	38 (15%)	4	6
1	C	261/261 (100%)	234 (90%)	27 (10%)	9	16
2	B	129/136 (95%)	115 (89%)	14 (11%)	8	14
2	D	129/136 (95%)	116 (90%)	13 (10%)	9	17
All	All	780/794 (98%)	688 (88%)	92 (12%)	6	12

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	17	ARG
1	A	24	LEU
1	A	35	GLN
1	A	53	THR
1	A	56	ARG
1	A	58	SER
1	A	59	PHE
1	A	65	ARG
1	A	74	SER
1	A	78	ASN
1	A	79	THR
1	A	81	LEU
1	A	84	LYS
1	A	113	ARG
1	A	116	THR
1	A	119	SER
1	A	134	HIS

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Mol	Chain	Res	Type
1	A	151	ARG
1	A	213	SER
1	A	229	ARG
1	A	232	LYS
1	A	235	LEU
1	A	236	ASP
1	A	237	PRO
1	A	238	SER
1	A	243	VAL
1	A	244	LYS
1	A	255	HIS
1	A	269	ARG
1	A	270	VAL
1	A	272	GLU
1	A	285	TYR
1	A	287	GLN
1	A	296	ARG
1	A	302	LEU
1	A	305	ASN
1	A	310	LEU
2	B	10	GLU
2	B	30	LEU
2	B	32	LEU
2	B	46	LEU
2	B	55	ARG
2	B	56	LYS
2	B	69	ASP
2	B	87	ASP
2	B	88	ASN
2	B	98	SER
2	B	101	GLU
2	B	106	VAL
2	B	112	SER
2	B	153	ASN
1	C	12	ILE
1	C	59	PHE
1	C	65	ARG
1	C	74	SER
1	C	84	LYS
1	C	97	THR
1	C	105	ARG
1	C	108	GLN

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Mol	Chain	Res	Type
1	C	136	THR
1	C	147	GLN
1	C	151	ARG
1	C	216	GLU
1	C	218	VAL
1	C	228	THR
1	C	229	ARG
1	C	231	GLN
1	C	233	GLU
1	C	234	ARG
1	C	236	ASP
1	C	252	SER
1	C	269	ARG
1	C	279	LYS
1	C	285	TYR
1	C	296	ARG
1	C	299	LEU
1	C	306	ARG
1	C	310	LEU
2	D	10	GLU
2	D	39	ASP
2	D	41	ARG
2	D	43	THR
2	D	87	ASP
2	D	90	GLU
2	D	95	SER
2	D	96	ARG
2	D	121	VAL
2	D	123	SER
2	D	128	ARG
2	D	132	ASN
2	D	153	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	21	ASN
1	A	78	ASN
1	A	106	HIS
1	A	170	HIS
1	A	212	HIS

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Mol	Chain	Res	Type
1	A	282	HIS
1	A	287	GLN
1	A	297	GLN
2	B	40	GLN
2	B	47	ASN
2	B	105	ASN
2	B	117	HIS
1	C	8	HIS
1	C	60	GLN
1	C	106	HIS
1	C	134	HIS
1	C	156	HIS
1	C	170	HIS
1	C	282	HIS
1	C	291	ASN
1	C	297	GLN
2	D	73	GLN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - 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
4	CTP	B	155	-	21,30,30	2.71	10 (47%)	31,47,47	2.47	10 (32%)
4	CTP	D	155	2	21,30,30	2.78	10 (47%)	31,47,47	2.54	9 (29%)

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
4	CTP	B	155	-	-	0/18/38/38	0/2/2/2
4	CTP	D	155	2	-	0/18/38/38	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	155	CTP	C3'-C4'	-5.36	1.38	1.53
4	B	155	CTP	C3'-C4'	-5.20	1.39	1.53
4	D	155	CTP	PG-O3G	-3.00	1.43	1.54
4	B	155	CTP	PG-O3G	-2.52	1.45	1.54
4	D	155	CTP	PA-O5'	-2.31	1.48	1.59
4	B	155	CTP	PA-O5'	-2.30	1.48	1.59
4	D	155	CTP	C4-N4	-2.21	1.28	1.35
4	B	155	CTP	PG-O1G	-2.12	1.44	1.51
4	B	155	CTP	C5-C4	2.09	1.45	1.40
4	D	155	CTP	C5-C4	2.45	1.46	1.40
4	B	155	CTP	O5'-C5'	3.01	1.57	1.44
4	D	155	CTP	O5'-C5'	3.02	1.57	1.44
4	D	155	CTP	O3'-C3'	3.76	1.52	1.43
4	D	155	CTP	O4'-C4'	3.94	1.54	1.45
4	B	155	CTP	O4'-C4'	4.03	1.54	1.45
4	B	155	CTP	O3'-C3'	4.40	1.53	1.43
4	D	155	CTP	O4'-C1'	4.67	1.47	1.41
4	B	155	CTP	O4'-C1'	4.93	1.47	1.41
4	B	155	CTP	C6-N1	5.06	1.42	1.35
4	D	155	CTP	C6-N1	5.70	1.43	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	155	CTP	PB-O3B-PG	-5.61	113.85	132.67
4	B	155	CTP	O4'-C1'-N1	-4.83	97.89	108.08
4	B	155	CTP	PB-O3B-PG	-4.48	117.65	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	155	CTP	C5-C4-N3	-4.47	116.17	121.80
4	B	155	CTP	C5-C4-N3	-4.09	116.64	121.80
4	B	155	CTP	O4'-C4'-C3'	-3.38	98.34	105.15
4	D	155	CTP	O4'-C4'-C3'	-3.35	98.39	105.15
4	D	155	CTP	O4'-C1'-N1	-3.17	101.40	108.08
4	B	155	CTP	O3'-C3'-C4'	-2.81	102.64	111.05
4	B	155	CTP	C5-C6-N1	-2.30	114.94	120.58
4	D	155	CTP	C5-C6-N1	-2.22	115.15	120.58
4	B	155	CTP	O3G-PG-O1G	2.37	118.19	110.58
4	D	155	CTP	O3G-PG-O1G	2.42	118.36	110.58
4	D	155	CTP	C2-N3-C4	4.13	121.44	115.61
4	D	155	CTP	C5-C4-N4	4.25	127.82	121.31
4	B	155	CTP	C2-N3-C4	4.51	121.97	115.61
4	B	155	CTP	C5-C4-N4	4.67	128.46	121.31
4	B	155	CTP	C2'-C3'-C4'	6.18	115.32	102.61
4	D	155	CTP	C2'-C3'-C4'	7.76	118.55	102.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	155	CTP	7	0
4	D	155	CTP	6	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.