



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:01 PM GMT

PDB ID : 1W7P
Title : The crystal structure of endosomal complex ESCRT-II
(VPS22/VPS25/VPS36)
Authors : Teo, H.; Perisic, O.; Gonzalez, B.; Williams, R.L.
Deposited on : 2004-09-07
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

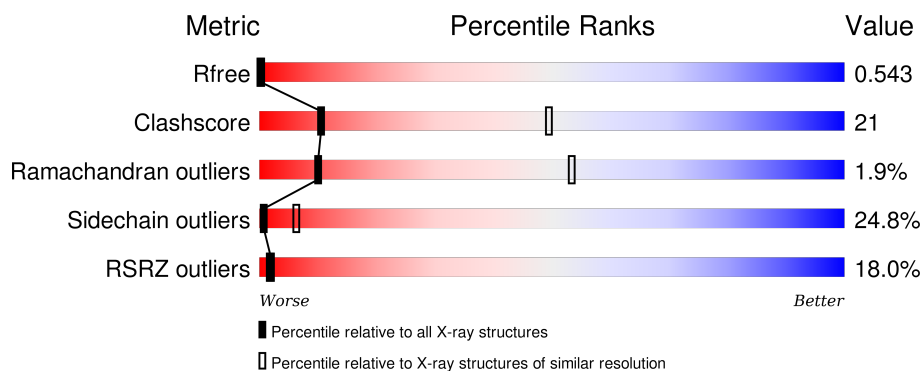
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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.

Mol	Chain	Length	Quality of chain
1	A	233	
2	B	202	
2	C	202	
3	D	566	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6134 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 VPS22, YPL002C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1732	1108	290	323	11			

- Molecule 2 is a protein called VPS25, YJR102C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	0	0	0
			1504	959	252	284	9			
2	C	182	Total	C	N	O	S	0	0	0
			1504	959	252	284	9			

- Molecule 3 is a protein called VPS36P, YLR417W.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	171	Total	C	N	O	S	0	0	0
			1394	891	226	268	9			

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.

Chain A:

Amino Acid	Category	Percentage
Met	Grey	16%
Lys	Green	52%
Gln	Green	52%
Phe	Green	52%
Gly	Green	52%
Leu	Green	52%
Ala	Green	52%
Phe	Green	52%
Asp	Green	52%
Glu	Green	52%
Leu	Green	52%
Lys	Green	52%
Tyr	Green	52%
Asn	Green	52%
Asp	Green	52%
V20	Green	52%
M21	Green	52%
I24	Green	52%
L25	Green	52%
Q28	Green	52%
S29	Green	52%
V30	Green	52%
R33	Yellow	33%
D34	Yellow	33%
E41	Yellow	33%
V44	Yellow	33%
K47	Yellow	33%
K48	Yellow	33%
N51	Yellow	33%
L54	Yellow	33%
Q55	Yellow	33%
E59	Yellow	33%
F60	Yellow	33%
H66	Yellow	33%
I73	Yellow	33%
D74	Yellow	33%
P75	Yellow	33%
L76	Yellow	33%
S77	Yellow	33%
L78	Yellow	33%
F79	Yellow	33%
R80	Yellow	33%
D81	Yellow	33%
R84	Yellow	33%
H85	Yellow	33%
F86	Yellow	33%
T87	Yellow	33%
N89	Yellow	33%
D90	Yellow	33%
F91	Yellow	33%
Y92	Yellow	33%
Y93	Yellow	33%
F94	Yellow	33%
V95	Yellow	33%
C96	Yellow	33%
K98	Yellow	33%
V99	Yellow	33%
I100	Yellow	33%
E101	Yellow	33%
T106	Yellow	33%
K107	Yellow	33%
D108	Yellow	33%
M109	Yellow	33%
N110	Yellow	33%
G111	Yellow	33%
G112	Yellow	33%
V113	Yellow	33%
I114	Yellow	33%
E118	Yellow	33%
I119	Yellow	33%
E120	Yellow	33%
K121	Yellow	33%
F124	Yellow	33%
R125	Yellow	33%
K126	Yellow	33%
L127	Yellow	33%
N128	Yellow	33%
L131	Yellow	33%
D132	Yellow	33%
D133	Yellow	33%
D139	Yellow	33%
M140	Yellow	33%
S143	Yellow	33%
C146	Yellow	33%
F147	Yellow	33%
Q151	Yellow	33%
I152	Yellow	33%
K153	Yellow	33%
G154	Yellow	33%
L158	Yellow	33%
K159	Yellow	33%
S160	Yellow	33%
V161	Grey	9%
P162	Grey	9%
P163	Grey	9%
E164	Grey	9%
L165	Grey	9%
T166	Grey	9%
S167	Grey	9%
D168	Grey	9%
S169	Grey	9%
Q169	Grey	9%
T170	Grey	9%
K171	Grey	9%
E174	Grey	9%
I175	Grey	9%
C176	Grey	9%
S177	Grey	9%
I178	Grey	9%
Y181	Grey	9%
S182	Grey	9%
S183	Grey	9%
I184	Grey	9%
S185	Grey	9%
L186	Grey	9%
L187	Grey	9%
N190	Grey	9%
L191	Grey	9%
C192	Grey	9%
M193	Grey	9%
R197	Grey	9%
S198	Grey	9%
K199	Grey	9%
S200	Grey	9%
E201	Grey	9%
L202	Grey	9%
L210	Grey	9%
L213	Grey	9%
E214	Grey	9%
Y215	Grey	9%
Q216	Grey	9%
G217	Grey	9%
E220	Grey	9%
E221	Grey	9%
L222	Grey	9%
Y223	Grey	9%
W224	Grey	9%
S227	Grey	9%
W228	Grey	9%
I229	Grey	9%
T230	Grey	9%
R231	Grey	9%
Q232	Grey	9%
Leu	Grey	9%

Chain B:

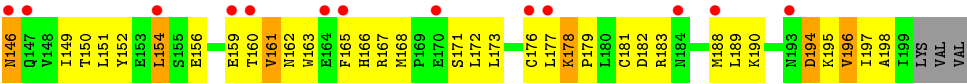
16% 38% 40% 12% 10%

Amino Acid	Category
W138	W
F139	F
E140	E
D141	D
L145	L
V148	V
I149	I
T150	T
L151	L
Y152	Y
E153	E
L154	L
S155	S
E156	E
E159	E
T160	T
V161	V
M162	M
V163	V
F164	F
P165	P
H166	H
R167	R
M168	M
P169	P
E170	E
S171	S
L172	L
L173	L
G176	G
L177	L
K178	K
P179	P
L180	L
C181	C
R185	R
A186	A
L187	L
M188	M
L189	L
K190	K
D191	D
D194	D
K195	K
V196	V
L197	L
A198	A
I199	I
LYS	L
VAL	V
VAL	V
LYS	L
I1E	I
S1E	S
K73	K
N74	N
L75	L
F76	F
N77	N
N78	N
E79	E
D80	D
I81	I
Q82	Q
R83	R
S84	S
F89	F
I90	I
D91	D
S95	S
Q96	Q
N97	N
T98	T
K99	K
E100	E
G101	G
K102	K
C103	C
L104	L
P105	P
I106	I
D107	D
Q108	Q
S109	S
G110	G
R111	R
R112	R
S113	S
S114	S
T117	T
T118	T
T119	T
R120	R
Y121	Y
F122	F
I123	I
L124	L
W125	W
D129	D
S130	S
W131	W
A132	A
S133	S
L134	L
I135	I
L136	L
G137	G
M1	M
S2	S
A3	A
L4	L
P5	P
F6	F
V7	V
Y8	Y
S9	S
F10	F
P11	P
P12	P
L13	L
Y14	Y
T15	T
R16	R
N19	N
T22	T
R23	R
R24	R
Q25	Q
Q26	Q
L27	L
S28	S
T29	T
W30	W
I34	I
S35	S
Q36	Q
Y37	Y
C38	C
K39	K
T40	T
K41	K
K42	K
I43	I
W44	W
T51	T
V52	V
I53	I
N54	N
ASP	A
ASN	A
GLU	G
LEU	L
ASP	A
SER	S
GLY	G
SER	S
THR	T
ASP	A
ASN	A
ASP	A
ASP	A
SER	S
LYS	L

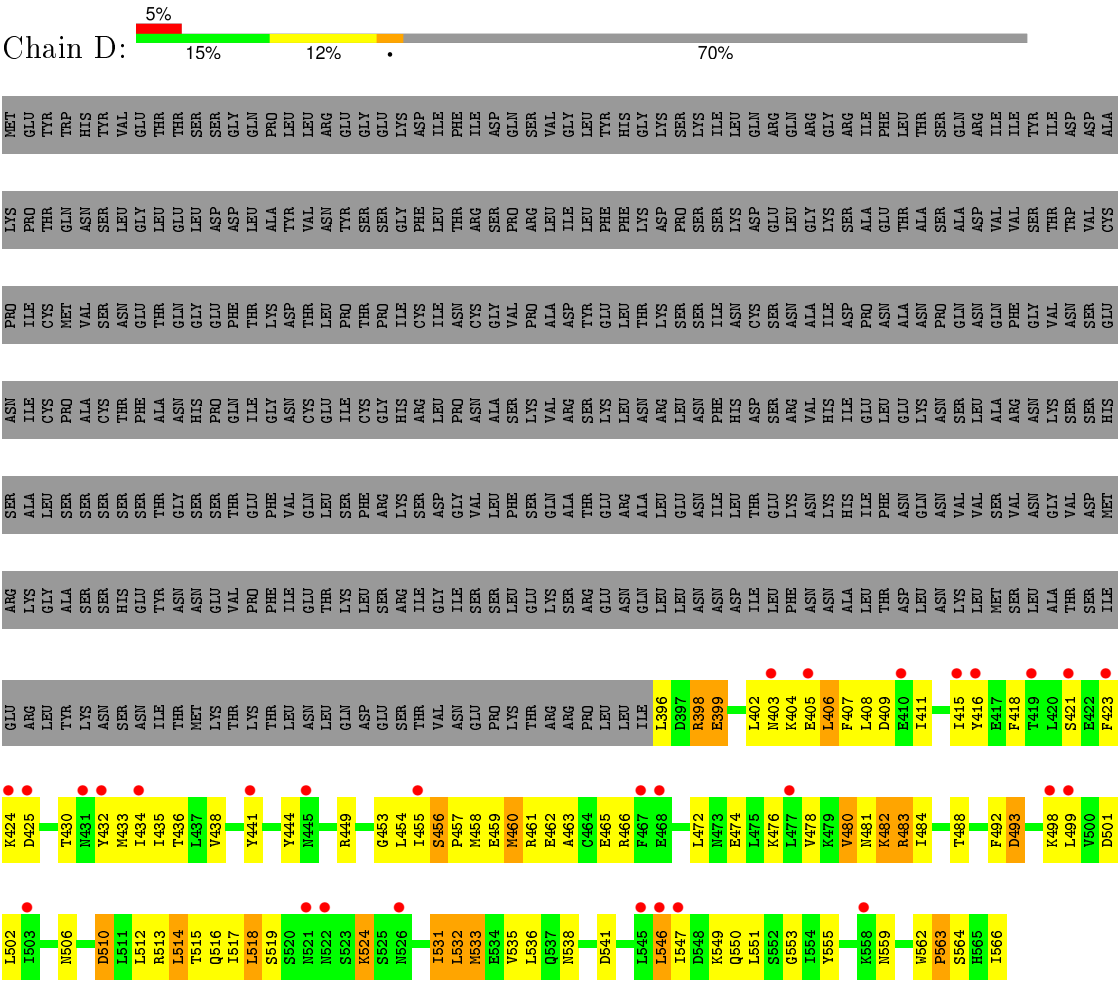
Chain C:

18% 38% 39% 11% 10%

M1 S2 A3 L4 P5 F6 V7 P11 P12 L13 R16 Q17 R23 R24 Q25 Q26 W30 I31 D32 D32 I33 I34 S35 Q36 Y37 C38 K41 K42 Y45 K46 D49 G50 T51 R52 I53 H54 ASP ASN GLU LEU SER ASP GLY THR ASN ASP ASP SER LYS LYS TLE S72



● Molecule 3: VPS36P, YLR417W



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	149.91Å 149.91Å 186.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.06 – 3.60 92.11 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (92.06-3.60) 99.0 (92.11-3.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.292 , 0.330 0.529 , 0.543	Depositor DCC
R_{free} test set	1216 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	141.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 174.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25002 reflections	Xtriage
F_o, F_c correlation	0.50	EDS
Total number of atoms	6134	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.80	0/1764	0.88	6/2372 (0.3%)
2	B	0.68	0/1539	0.91	5/2087 (0.2%)
2	C	0.75	0/1539	0.94	5/2087 (0.2%)
3	D	0.85	0/1416	0.95	4/1908 (0.2%)
All	All	0.77	0/6258	0.92	20/8454 (0.2%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	425	ASP	CB-CG-OD2	7.14	124.73	118.30
1	A	168	ASP	CB-CG-OD2	6.91	124.52	118.30
2	C	107	ASP	CB-CG-OD2	6.73	124.36	118.30
3	D	501	ASP	CB-CG-OD2	6.44	124.09	118.30
3	D	510	ASP	CB-CG-OD2	6.43	124.09	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1732	0	1741	51	0
2	B	1504	0	1487	80	0
2	C	1504	0	1487	93	0
3	D	1394	0	1406	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6134	0	6121	262	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 21.

The worst 5 of 262 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)
2:C:74:ASN:O	2:C:78:ASN:HB3	1.46	1.16
2:C:94:TRP:CE2	2:C:121:TYR:CD2	2.58	0.92
2:C:122:PHE:CZ	2:C:172:LEU:HD22	2.06	0.90
2:B:186:ALA:HB1	2:B:199:ILE:HA	1.57	0.86
2:C:122:PHE:CE2	2:C:172:LEU:HD22	2.11	0.84

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	211/233 (91%)	188 (89%)	22 (10%)	1 (0%)	34 77
2	B	178/202 (88%)	144 (81%)	28 (16%)	6 (3%)	5 41
2	C	178/202 (88%)	148 (83%)	24 (14%)	6 (3%)	5 41
3	D	169/566 (30%)	145 (86%)	23 (14%)	1 (1%)	30 74
All	All	736/1203 (61%)	625 (85%)	97 (13%)	14 (2%)	10 53

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	16	ARG
2	C	78	ASN

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Mol	Chain	Res	Type
3	D	563	PRO
2	B	81	ILE
2	B	101	GLY

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	195/211 (92%)	149 (76%)	46 (24%)	1	7
2	B	173/192 (90%)	134 (78%)	39 (22%)	1	8
2	C	173/192 (90%)	127 (73%)	46 (27%)	0	5
3	D	160/519 (31%)	117 (73%)	43 (27%)	0	4
All	All	701/1114 (63%)	527 (75%)	174 (25%)	1	6

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	171	SER
2	C	78	ASN
3	D	512	LEU
2	B	187	THR
2	C	25	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	96	GLN
2	B	193	ASN
3	D	403	ASN
2	B	74	ASN
3	D	431	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](#)

There are no ligands in this entry.

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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	213/233 (91%)	1.34	37 (17%) 2 2	57, 60, 61, 62	0
2	B	182/202 (90%)	1.07	33 (18%) 2 2	57, 60, 61, 62	0
2	C	182/202 (90%)	0.93	36 (19%) 1 1	58, 60, 61, 63	0
3	D	171/566 (30%)	1.04	29 (16%) 2 2	57, 59, 61, 62	0
All	All	748/1203 (62%)	1.11	135 (18%) 2 2	57, 60, 61, 63	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	109	SER	8.8
2	B	40	THR	5.9
3	D	432	TYR	5.6
3	D	441	TYR	5.2
2	B	176	CYS	5.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.